Lecture Notes for Quantum Matter

MMathPhys

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Contents

Preface

This course covers interesting quantum states of matter: Superfluids, Superconductors, and Fermi Liquids. This is where condensed matter really starts to get bizarre — and therefore even more fun (at least in my opinion).

I realize that possibly not everyone will have actually attended the official prerequisite courses (or possibly did attend, but didn't pay attention), so I will try to make this course as self-contained as possible, while still making contact with what has been taught in prior courses.

Particularly for those who have read the *Oxford Solid-State Basics*, I will warn you right from the front that this book is higher level and is likely to be more difficult going. Whereas that book was written as a third year undergrad course, this book is written at a masters level for students who have a good amount of theoretical background already.

Lets get started!

At early points in one's career there is an inevitable tension between learning physics and learning mathematical formalism. While learning to manipulate commutation relations, and even learning the rules for green's function expansions can be fun — and indeed, by doing this one gets a feeling that one is actually learning something — the real hard part is learning to develop intuition for physics. Developing intuition is extremely hard, and it is something that professional physicists struggle with throughout their lives.

This course needs to strike a balance between the two tasks. For some we will not learn enough formalism. For others we will not learn enough physics. I hope we will be able to satisfy both factions, and I hope everyone will learn at least a bit of both.

Chapter 1

What we will study

1.1 Bose Superfluids (BECs, Superfluid He, Superconductors)

Much of the term will be focused on discussion of superfluids and superconductors.

We will discuss both Bose Einstein Condensates (BECs) and superfluids — the main example being superfluid Helium 4. The difference here is that a BEC is by definition a gas of noninteracting bosons, whereas Helium 4 is strongly interacting. In the modern era one calls a weakly interacting Bose gas a BEC also – since it can be treated as a weak perturbation of the noninteracting case. Helium 4, however, is very far from noninteracting.

The tension between the physics of the interacting and noninteracting cases will be a theme.

We will then turn to the study of superconductors. First we will view these as simply being a superfluid of charged bosons.

Of course superconductors are things like aluminum[1] are regular metals, where the charged objects are electrons, which are fermions of charge $-e$. However, as we will see later, these charged objects can pair into bosons of charge $-2e$.

Why are such pairs bosons? Recall that fermions accumulate a minus sign when they are exchanged. Exchanging a pair of fermions with another pair of fermions accumulates an even number of minus signs, hence a plus sign, so the pair of fermions is a boson.

This picture of electrons pairing into bosons is not entirely accurate and there are good reasons to believe that even using this as a cartoon picture is quite dangerous. However, in some other ways this picture does make sense. In order to figure out how it makes sense we must first take a detour into a study of Fermions.

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[1] Those using the british spelling and pronounciation "aluminium" will be ridiculed.

1.2 Theory of Fermi Liquids

Fermi liquids, metals and other systems of interacting fermions have some unusual properties — some of which you have probably studied in your introductory solid state or condensed matter courses[2]. However, in most of these treatments, the interaction between fermions is completely neglected. This is a terrible thing to do being that the interaction energy scale is usually just as a big (and sometimes even bigger) than the Fermi energy — and both are immensely bigger than the temperature for usual metals at room tempertature. We will need to understand some of the properties of these Fermi systems before we can go on to understand the more exotic physics of electron pairing.

1.3 BCS theory of superconductivity

This is not examinable

1.4 Special topics

also not examined. Subjects we may cover include:

Integer quantum Hall effect.

Topological Insulators.

Majoranas

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[2] If you have not studied introductory solid state physics, you should do so. I can recommend a good book.

Chapter 2

Introduction to Superfluids

Superfluids and superconductors share the unusual property of zero dissipation. For example, we can imagine a toroidal pipe which we can fill with ^{4}He. If we start ^{4}He supefluid flowing around the torus it will continue essentially forever (with caveats that T must be low enough, the velocity must be small enough, and the system must be big enough). "Forever" here means an essentially unmeasurable long time.

Similarly with a superconductor. we can take a solid torus (a very thick loop of wire) and if we start a current flowing around the wire , it will conitnue with no loss essentially forever (again caveats, the temperature must be low enough, the current must be small enough and the the sample must be big enough). Experiments have measured that the decay time in certain superconducting wires exceeds 10^5 years. It is probably much longer, but it becomes very difficult to measure such tiny amounts of decay.

Insert story about crazy Gerrit Flim demonstrating persistant current flow in superconductors.

2.1 Some History and Basics of Superfluid Phenomena

In 1908 in Leiden, Heike Kamerlingh Onnes liquified helium for the first time allowing access to extremely low temperatures.

On April 8, 1911 Kamerlingh Onnes "discovered" both supercondctivity and superfluidity.

He noticed that below 4.2K the resistance of mercury (Hg) metal suddenly becomes unmeasurably small. He spent the next few years convincing himself that this is a real effect and not some error in the experiment. He also shows that many metals have the same superconducting behavior — each with its own critical temperature. There was no real explanation of the observed superconductivity until 1957 (the BCS theory). We will discuss superconductivity more in later chapters, but this chapter will focus on superfluidity.

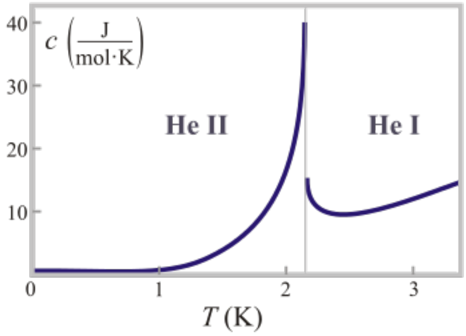

Figure 2.1: The Lambda transition in helium. The superfluid phase is known as He II.

On the very same day as the discovery of superconductivity, he notes in his lab book that something different is happening around 2K, but he didn't follow up on this for many years.

In 1913 Kamerlingh Onnes wins the Nobel prize.

In 1922-23 Onnes, along with some of his coworkers goes back to re-examine the "something strange" that happens around 2K. Looking at the heat capacity, they find something like Fig. 2.1. The discontinuity in the heat capacity is a signal of a thermodynamic phase transition[1] The regular phase of helium is known as He I whereas[2] the superfluid phase is known as He II.

Onnes died in 1926, but the work in his lab continued on. With some exploration, they uncovered the full phase diagram shown in Fig. 2.2. The line separating the He I and He II phases is known as the Lambda-line.

Compared to other elements, helium is quite special in that it does not solidify at low temperature except when under pressure. This special feature is due to both its very light mass and its weak interactions (no chemical bonding). The light mass is important since $\Delta p \Delta x \geqslant \hbar/2$. If you try to localize x, you have a nonzero p. But since kinetic energy is $p^2/(2m)$ having a light mass means there is a very high energy cost to localizing the position of the atoms.

The most remarkable thing about superfluid helium is persistant flow (which Kamerlingh Onnes was never aware of). However, perhaps just as remarkable is the extremely good transport of heat in superfluids. In fact, going through the supefluid transition, ther-

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[1] For those who have studied phase transitions we have $C_v \sim B_\pm + A_\pm |T - T_c|^{-\alpha}$ where the critical exponent $\alpha \approx -0.0127$ matches that of the XY-universality class and here $A_\pm$ and $B_\pm$ are different constants depending on whether we approach the critical point from the high or low temperature direction. When we study the order parameter in section 2.3 it will be clear to those having studied phase transitions wwhy this is in the XY universality class.

[2] This nomenclature is particularly confusing being that we also have ^{4}He and ^{3}He, indicating the number of nucleons. Everything in this chapter is in reference to phases of regular helium, ^{4}He, although we will also discuss ^{3}He in our chapter below on Fermi liquids.

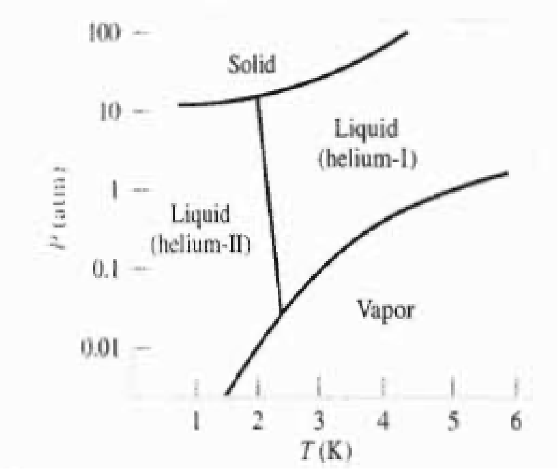

Figure 2.2: The Phase Diagram (P,T) of ^{4}He. The superfluid phase is known as He II. The nonsuperfluid phase is known as He I

mal conductance can jump by a factor of 10^5 or more! Indeed, this was what Kamerlingh Onnes saw in 1911 when he said "something happens" at 2K). What is happening here is that the fluid suddenly goes from rapid boiling to no boiling at all in the superfluid phase. Boiling occurs when a small region of a system is at slightly higher temperature than the vaporization transition. This region turns into gas and then boils up to the top of the containier. In a superfluid, the thermal transport is so good that no region in the sample is at higher temperature than any other region. The system still has evaporation, but only directly from the surface.

The discovery of the superfluid properties of He II did not come until the mid 1930s. The next heros of our story are Peter (Pyotr) Kapitsa and John Allen.

Peter Kaptiza, having survived the flu epidimeic of 1918-19 in Russia which claimed half of his family, had moved to Cambridge to study with Rutherford. He was made a fellow of Trinity College Cambridge in 1925 two years after obtaining his PhD and he went on to build one of the world's finest low temperature physics labs at Cambridge. By the mid 1930s Kaptiza was earning what was considered a magnificent salary of 800 pounds per year.

By the early 1930s there were only four labs in the world that were able to liquidify helium and conduct low temperature experiments: Leiden, Oxford[3], Cambridge, and Berlin.

John Allen received his PhD from Toronto in their cryogenics lab, and moved to Cambridge to work with Kaptiza. Unfortunately, when he arrived there, he discovered that Kapitsa had been "detained" on a visit to the Soviet Union, and was told that he

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[3] Oxford had liquid helium in 1933, one year before Cambridge did. Fredrick Lindemann, the first Viscount Cherwell, advertised Oxford's success in the Times and Nature. Nonetheless, the crucial discovery of superfluid flow was made at Cambridge

would not be allowed to return to Cambridge. This was the era of Stalin, and the Soviets wanted to have the great Kaptiza back in his native land.

Kaptiza was well funded by the Soviets to set up a low temperature physics lab (they purchased much of his equipment from Cambridge).

John Allen, at Cambridge with no supervisor, had to work as an unsupervised postdoc. Rutherford, the head of the Cavendish lab at Cambridge, made the best of the situation — he used Kaptiza's salary to pay both Allen and a young theorist named Rudolf Peierls.

The cryogenic race was on: it was clear that there was plenty of interesting physics to be discovered to whoever got there first!

In 1938 both Kaptiza and Allen (with Misener, another student from the Toronto lab) simultaneously discovered the effect that gives superfluid helium its name — that superfluid helium flows with apparently no resistance through very thin capillaries.

Another very strange effect, now known as supercreep, was discovered the following year in Oxford by Sir Francis Simon (no relation that I know of) and Bernard Rollin: Superfluid helium in an open-topped container will creep up the walls of the container and eventually find its way to lower gravitational potential by siphoning itself onto the floor. This effect is often viewed as a combination of wetting and zero viscosity. Many liquids will form a layer an atom or two thick on the walls of their container all around the container — this is due to the attractive forces between the wall of the container and the fluid molecules. This phenomenon is known as wetting. Superfluid helium, with no viscosity, can flow readily through a layer which is atomically thin – whereas other fluids cannot. Thus superfluid helium can siphon itself out of a container onto the floor through this very thin layer.

However, the situation is more complicated than simply saying that the fluid has zero viscocity. Other experiments aiming the measure the viscocity of the liquid come up with finite results. For example, a vibrating wire, or rotating disk in the helium liquid will detect a finite viscous damping which only vanishes at zero temperature (Keesom and MacWood, Leiden Lab, 1938). This connundrum was one of the key points that led to the development of Landau's two fluid model.

2.2 Landau and the Two Fluid Model

2.2.1 More History and a bit of Physics

In 1938 just as Kapitsa was discovering superfluidity, the great theorist, Lev Landau was thrown in prison for publicly comparing Stalin to Hitler[4]. He remained imprisoned for a year until Kapitsa put his own head on the line — threatening to quit as a scientist unless Landau was released, and pleading that only Landau would be able to explain

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[4] He was exceedingly lucky not to have been executed!

superfluidity.

While Landau was in prison, the young Hungarian physicist Laszlo Tisza[5] working in Paris with Fritz London tried to explain superfluidity as a result of Bose-Einstein condensation[6]. Fritz and his brother Heinz London, several years earlier working with Lindemann in Oxford, had already tried to use a similar approach for understanding superconductors. While they had some success, Landau immediately realized what was wrong with their approach.

- Helium is *NOT* a noninteracting boson. It has extremely strong short range repulsive interactions.
- A noninteracting BEC does not have a discontinuity in its specific heat
- A noninteracting BEC will *NOT* superflow. Interactions are crucial for obtaining this effect. (We will explain this in detail below in section 2.4)

At this point Landau gets into the game. He felt that BEC was not the right physics[7] — perhaps he even felt this more strongly than is actually warranted. Later Feynmann would clarify the importance of Bose physics for superfluidity (See below in chapter 5).

Landau made two major contributions to the theory of superfluidity.

- He develops the two-fluid model (an expansion on Tisza's work)
- He explains the criterion for superflow.

These contributions earned Landau a Nobel prize in 1962.[8]. Sadly a few months before the prize was annouced, Landau was in a car crash and coma. While he came out of the coma, he never fully recovered, he was never scientifically productive again, and he died in 1968, at age 60, from complications due to these injuries.

2.2.2 Landau's Two Fluid Model

The general idea of the two fluid model is that we should imagine two interpenetrating fluids which we call "super" and "normal"[9]. We write the total density of the fluid as the sum of the mass densities of the super and normal fractions.

$$\text{mass/volume} = \rho_{total} = \rho_S + \rho_N.$$

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[5] Tisza moved to MIT in 1941 and lived in the US the remainder of his life. He passed away in 2009 at the age of 101.

[6] The prediction of BEC by Einstein was much earlier, in 1925.

[7] Apparently Landau also really hated Fritz London. It is unclear why this would be true, but Landau made a point never to cite London.

[8] There are many things that Landau could have been awarded a Nobel prize for!

[9] This is another terrible nomenclature. Above the critical temperature we have only normal fluid. But below the critical temperature we have both super and normal fluid. However, we also say that He II (below the critical temperature) is superfluid.

The normal fraction behaves like we should expect a fluid to behave. The superfluid fraction, however, has no viscosity, and carries no heat. At zero temperature we expect all of the fluid to be super, whereas above the critical temperature T_c, i.e., in the He I phase, we expect all of the fluid to be normal. At nonzero T but still in the He II phase, we expect to have a mixture of partially super and partially normal fluids.

$$\begin{array}{cccc} T = 0 & \rho_N = 0 & \rho_S = \rho & \\ T_c > T > 0 & \rho_N(T) & \rho_S(T) = \rho_{total} - \rho_N(T) & \text{interpolates} \\ T > T_c & \rho_N = \rho & \rho_S = 0 & \end{array}$$

One way to think about the super-fraction is to think of it as being the "ground state" of the system, and the normal fluid being the excitations. For a moment let us think about the analogy with BEC. In that system we know that only at $T = 0$ are all of the bosons in the same lowest energy eigenstate. At any finite T there will be some bosons in the lowest energy eigenstate (these we might call "super") and some will be in the excited eigenstaes (which we might call "normal"). Once we go above the critical temperature, there will a microscopic fraction of particles (essentially zero) in the lowest energy eigenstate, and the entire system will be normal.

The mass current will also be divided into a normal and super component

$$\mathbf{j} = \rho_S \mathbf{v}_S + \rho_N \mathbf{v}_N$$

with $\mathbf{v}_N$ being the normal fluid velocity and $\mathbf{v}_S$ being the superfluid velocity. Here the super part of the fluid will be free from viscosity but the normal part is not.

This two fluid model nicely "explains" the two different measurements of viscosity. With a vibrating wire or a rotating disk, the object moving through the fluid will have to push the normal fluid out of the way, and hence will measure the normal viscosity. However, when trying to push the fluid through a small capillary, no matter how thin the capillary, the super-fluid component will always flow through – whereas the normal fluid will stay behind. Since flow occurs through small capillaries one would measure a fluid with essentially zero viscosity.

From a technical standpoint the two fluid model actually imposes the curl-free constraint

$$\nabla \times \mathbf{v}_S = 0 \tag{2.1}$$

We will justify this constraint later; for now let us just treat it as a conjecture. However, it is worth understanding why this is an appropriate conjecture for a fluid that shows no visosity.

One explanation is to realize that viscosity is a statement transferring force through shear. However, the curl-free constraint is the statement that the fluid cannot shear at all! (Expand on this! add picture).

Suppose for a moment that ρ_S is fixed (say we are at zero temperature). Then we have

$$\nabla \cdot \mathbf{v}_S = 0$$

by current conservation. If we use our conjecture Eq. 2.1 we can use a vector identity to derive

$$\nabla^2 \mathbf{v}_S = \nabla(\nabla \cdot \mathbf{v}_S) - \nabla \times (\nabla \times \mathbf{v}_S) = 0$$

If we then recall the Navier-Stokes equation we have

$$\left[\frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla)\right] \mathbf{v} + \frac{1}{\rho} \nabla P = \frac{\eta}{\rho} \nabla^2 \mathbf{v}_S$$

where η is the coefficient of viscocity. By using the curl-free constraint the viscosity term always vanishes!

2.2.3 More Physical Effects and Their Two Fluid Pictures

Fountain Effect

Another strange effect observed by John Allen[10] is known as the "fountain effect", shown in the left of Fig. 2.3. A tube is inserted in the superfluid and plugged with cotton such that only the "super" fraction of the fluid can get through. Heating the cotton, will result in superfluid being sucked into the tube at a high rate such that it can fountain out the top. This effect was explained in 1939 by Heinz London[11] using the two-fluid model. In this picture we think of the motion of the fluid as being similar to osmosis. If in some region (such as in the tube) we increase the temperature from T to $T + \Delta T$, this increases the concentration of ρ_N. Using the usual principle of osmosis, this makes ρ_S flow into the hotter region to try to bring the normal fluid back ot the same concentration as that of the surrounding area. I.e., the superfluid flows into the hotter region to try to bring the temperature back down.

This physics may look like a violation of the 2nd law of thermodynamics since fluid is flowing from cold to hot. However, it is not a violation since the superfluid carries no heat.

The situation can be analyzed in more detail by using the experimental setup shown in the right of Fig. 2.3. Here the tube between the two containers is assumed to be plugged with cotton, or is such a thin capillary that only superfluid can flow through it (but not normal fluid). This is sometimes known as a "superleak."[12]

We can analyze the situation using simple thermodynamics. In particular, we use the Gibbs-Duheim relationship for the change in chemical potential which we set to zero

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[10] In fact, the discovery of this effect was a fortuitous error in an experiment!

[11] The London brothers were Jewish refugees from Germany in 1933. Lindeman at Oxford found money to fund as many German scientists as he could, but his money soon ran out. Fritz moved to Paris and eventually ended up at Duke university in the states. Heinz moved to Bristol, but was declared a potentially "hostile foreigner" and interned for some time on the Isle of Man. He was released to work on the British nuclear program and was given British citizenship. In the 1950s Heinz invented the dilution refrigerator which is used heavily in physics research for cooling materials down to as low as a few millikelvin.

[12] The superleak is crucial for this experiment since an open tube cannot have a pressure difference across it!

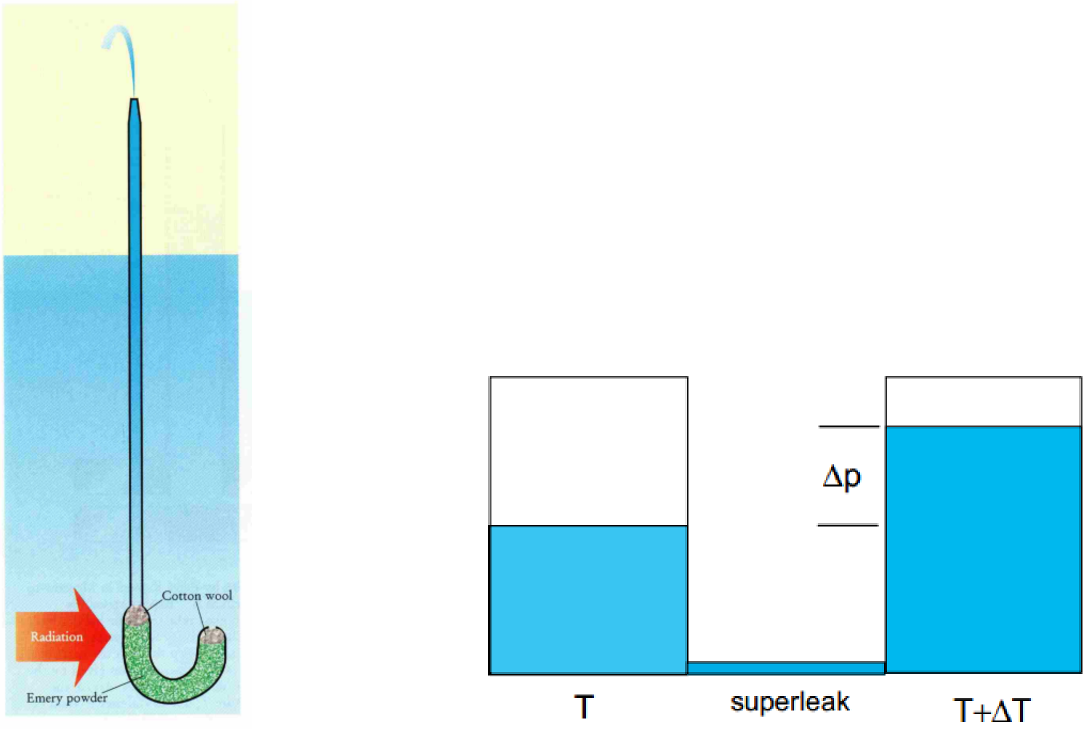

Figure 2.3: Left: The fountain effect. A tube is inserted in the superfluid and plugged with cotton such that only the "super" fraction of the fluid can get through. Heating the cotton, will result in superfluid being sucked into the tube at a high rate such that it can fountain out the top. Right: a similar experiment showing that a temperature difference implies a pressure difference.

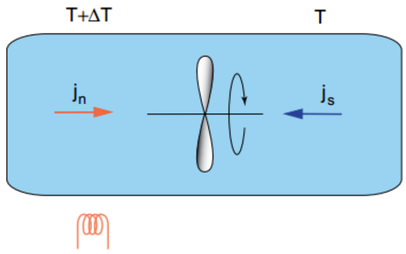

Figure 2.4: Thermomechanical Effect: The propeller turns as if fluid is flowing from hot to cold, even though there is no net tranport of mass.

in order to have equilibrium

$$d\mu = -\frac{S}{N}\,dT + \frac{V}{N}dP = 0$$

Rearranging this we can write

$$\frac{\Delta P}{\Delta T} = \frac{S}{V}$$

and the right hand side can be written in terms of

$$S(T) = \int_0^T dT' \frac{C_V(T')}{T'}$$

where C_V can be measured experimentally.

Thermomechanical Effect

In this experiment, a propeller is put in a container of helium. One side of the container is heated as shown in Fig. 2.4. No net current of fluid can flow due to the walls of the container. Nonetheless, the propeller turns as if fluid is flowing from hot to cold.

What is happening here is that the increased temperature (on the left in the figure) increases the density of normal fluid, and the normal fluid then tries to flow to the right. Similarly, by osmosis the superfluid tries to flow to the left to bring the two sides of the system into equilibrium where they have the same density of normal fluid (i.e., have the same temperature). Thus we have counter flow of normal and super fluid – with no net flow of mass.

Now the key is that the flow of the normal fluid pushes the propeller while the flow of the superfluid does not. The reason for this is that superfluid flow must not dissipate mechanical energy — otherwise superflow would not be dissipationless.

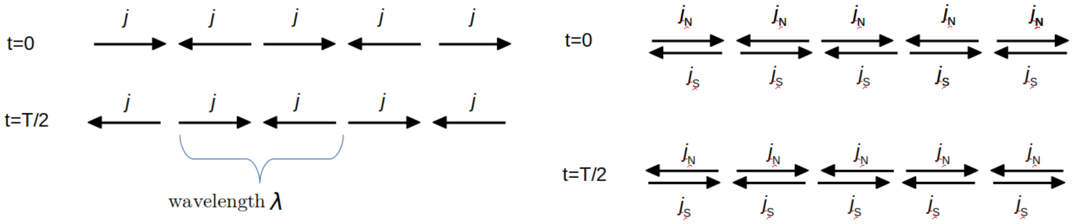

Figure 2.5: Left: Sound waves are density waves: mass sloshes back and forth. Right: Second sound waves involves counterflow. There is no mass transport, although heat is transported.

2.2.4 Second Sound

The idea of counter flow of normal and superfluids suggests the phenomenon of second sound[13].

First let us remind ourselves of how sound waves work. In the left of Fig. 2.5 we see the density flow in a sound wave — mass sloshes back and forth over the wavelength over the sound and with the period of the oscillation T. In the right of Fig. 2.5 we see second sound waves — the supercurrent is always counter-flowing the normal current so there is no net mass transport, $\mathbf{j}_{total} = 0$ everywhere. However, heat sloshes back and forth since only the normal current carries heat.

Such second sound waves provide extremely good thermal conduction — indeed, the best thermal conductance of any material since heat travels ballistically in second sound rather than diffusively. The heat transport can be over 100 times as efficient as heat transport in, say, copper.

Derivation of second sound

We now turn to do a more formal derivation of second sound. Since we are not interested in regular sound waves, we will assume that the pressure is constant and the density is constant (these approximations simplify quite a bit, but are not entirely necessary).

Since we have fixed density and fixed pressure, we will enforce

$$\mathbf{j}_{tot} = 0 = \rho_N \mathbf{v}_N + \rho_S \mathbf{v}_S$$

We now assume that there is an osmotic force from temperature imbalance. This is precisely the force that arises from the fountain effect. Usually we think of this as a force pushing the superfluid towards the heat, but since the total mass current is fixed to be zero, we can just as well think of this as a force pushing the normal fluid towards lower

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[13] Second sound was first predicted by Tisza. The correct second sound velocity was predicted by Landau.

temperature regions

$$\dot{\mathbf{v}}_N = -\alpha \nabla T \tag{2.2}$$

with $\alpha > 0$. It is a homework exercise to estimate the value of the coefficient α.

We now write a continuity equation for entropy. Let us write s for the entropy density. We then have a conservation equation

$$\dot{s} = -\nabla(s\mathbf{v}_N) \tag{2.3}$$

since the entropy moves with the normal fluid only (the super fraction contains no entropy).

The entropy density is a function of the local temperature, which we can expand

$$s(T + \delta T) = s(T) + \kappa \delta T$$

where recalling that $c_V = T ds/dT|_V$. we must have

$$\kappa = c_V(T)/T$$

Here c_V is heat capacity per unit mass.

We can now put this expansion of the entropy into Eq. 2.3 to obtain

$$\kappa \dot{T} = -s(\nabla \cdot \mathbf{v}_N)$$

Here it may look like there should be another term on the right which would be $\mathbf{v}_N \cdot \nabla s$. However, we can throw this out since this is second order in “small” things. I.e, the gradient of the temperature is assumed small and the velocity is also assumed small.

Differentitating with respect to time we obtain

$$\ddot{T} = -\frac{s}{\kappa} \nabla \cdot \dot{\mathbf{v}}_N = \left(\frac{s}{\kappa}\alpha\right) \nabla^2 T$$

where we have again thrown away terms second order in “small”, and we have also used Eq. 2.2. Thus we obtain the wave equation[14]

$$\ddot{T} = \gamma \nabla^2 T$$

with $\gamma > 0$ which tells us that heat propagates ballistically rather than diffusively as it usually does.

2.2.5 Big Questions Remaining

These questions will be addressed in the next sections.

1. What justifies the curl free constaint on the supercurrent $\nabla \times \mathbf{v}_S = 0$.

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[14] Using the homework assignment where we estimate α as well as some results later about C_V and ρ_N we can get that the second sound velocity is independent of T at low enough T.

2. Why do we get dissipationless superflow? This is *NOT* only a result of item (1) the curl free constraint.

3. What do we expect the normal/super fluid density to be as a function of temperature $\rho_N(T)$ and $\rho_S(T)$?

2.3 Curl Free Constraint: Introducing the Superfluid Order Parameter

One of Landau's other great contributions to physics is the concept of an *order parameter*. (If you have studied the Landau theory of phase transitions you will know what this is.) Roughly, the order parameter describes the breaking of a symmetry in a physical system.

As a simpler example, let us reconsider a BEC. In this case, we take the the order parameter to be the complex wavefunction for the ground state, which we write as ψ, however, we normalize it so that it goes to zero at the phase transition — i.e., it's amplitude is proportional to the number of bosons in the ground state.

What symmetry has been broken when going from the normal state above the critical temperature to the superfluid state below the critical temperature? It is actually a gauge symmetry! When the order parameter ψ becomes nonzero it must choose a complex phase, which is a spontaneous breaking of a symmetry!

In the case where the bosons are not uniform in space, we generalize the uniform Landau order parameter to a Landau-Ginzburg order parameter and write it as a function of position $\psi(\mathbf{r})$.

For interacting bosons we do something quite similar, we define an order parameter as

$$\psi(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle$$

where $\hat{\psi}(\mathbf{r})$ is a boson annihilation operator. We will be more explicit about this approach in later chapters 4. For now it is acceptable to just think of this order parameter as being the complex wavefunction of a BEC with the one complication that we want to change the normalization so that

$$\int d\mathbf{r} |\psi(\mathbf{r})|^2 = N_0$$

rather than normalization to unity. Here N_0 is the number of bosons in the condensate[15].

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[15] It is unfortunately not generally true that N_0/N is the same as the superfluid fraction from the two-fluid model in the case of an interacting Bose system. In the two-fluid model ρ_S is defined in terms of the amount of mass that flows with no dissipation — which at $T = 0$ is always the total mass of the fluid. However for interacting bosons the magnitude of the order parameter, which describes the number of particles in the condensate, will not be the full mass of the fluid even at $T = 0$. This will be more clear later when we give more rigorous definitions of the order parameter, and indeeed we calculate N_0 for a weakly interacting Bose gas in section 4.5 below.

We can separate the phase degree of freedom from the magnitude by writing

$$\psi(\mathbf{r}) = \sqrt{n_0}\, e^{i\theta(\mathbf{r})} \tag{2.4}$$

where $n_0 = N_0/N$ is the condsensate number density and θ is a phase defined modulo 2π. Here we can think of $e^{i\theta}/\sqrt{V}$ as being the usual normalization of the wavefunction of a boson in its ground state.

Again thinking of ψ as a wavefunction for superfluid bosons, then we can write the condensate current in the usual quantum mechanical way

$$\begin{aligned} \mathbf{j}_0 &= \frac{1}{2}\left(\psi^* \hat{\mathbf{p}}\psi - (\hat{\mathbf{p}}\psi^*)\psi\right) \\ &= \frac{-i\hbar}{2}\left(\psi^* \nabla\psi - (\nabla\psi^*)\psi\right) \end{aligned} \tag{2.5}$$

where here the momentum operator $\hat{\mathbf{p}}$ gives us a mass current.

Now using Eq. 2.4 we have

$$\nabla\psi = \left(\frac{\nabla n_0}{2n_0} + i\nabla\theta\right)\psi$$

which gives us a superfluid mass current of

$$\mathbf{j}_0 = \hbar n_0 \nabla\theta \tag{2.6}$$

We can write this current as a mass density times a superfluid velocity

$$\mathbf{j}_0 = \rho_0 \mathbf{v}_S$$

which, using $\rho_0 = m n_0$ gives us an expression for the superfluid velocity[16]

$$\mathbf{v}_S = \frac{\hbar}{m}\nabla\theta$$

which is a gradient. This then implies the desired curl-free constraint

$$\nabla \times \mathbf{v}_S = 0$$

2.3.1 Vorticity Quantization

Circulation is defined as the line integral of a velocity around a closed contour. Choosing any given closed contour we have

$$\oint_C \mathbf{v}_S \cdot \mathbf{dl} = \frac{\hbar}{m}\oint_C \nabla\theta \cdot \mathbf{dl} = 2\pi p\hbar/m = ph/m \tag{2.7}$$

---

[16] Although as mentioned above in footnote 15 the condensate fraction n_0 may not match the superfluid fraction of the two-fluid model, it is nonetheless true that both pictures give the same expression for the supefluid velocity.

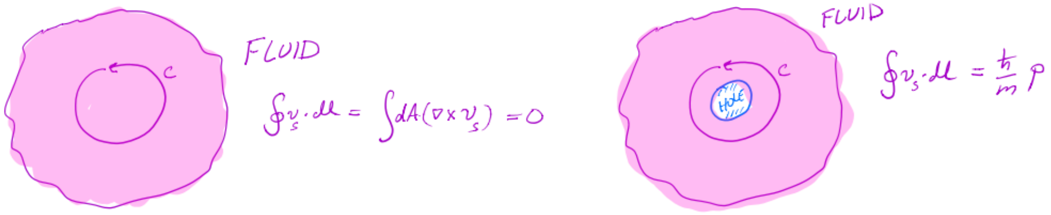

Figure 2.6: Left: A contour in fluid that can be contracted and therefore bounds a disk in the fluid. In this case the circulation must be zero. Right: A contour in fluid that cannot be contracted. In this case we can only say that the circulation is quantized in units of the elementary circulation quantum h/m.

where p is an integer. Here we have used the fact that θ must be well defined only modulo 2π so going around a closed path, the value of θ needs to come back to the same value, but can change by integer multiples of 2π.

Thus we have shown that in a superfluid circulation is quantized in integer multiples of the circulation quantum h/m.

Suppose now that our contour surrounds only He fluid as shown in the left of Fig. 2.6. I.e, we have a big sample of He fluid [with nothing else in it but He fluid] and the contour can be continously contracted to a point. In this case we can use Stoke's theorem

$$\oint_{C=\partial D} \mathbf{v}_S \cdot \mathbf{dl} = \int_D dA \cdot (\nabla \times \mathbf{v}_S) = 0$$

where the area integration is over a disk D bounded by the contour C. Thus we would conclude that the circulation must be zero. However, this conclusion is only true if superfluid fills the entire disk. If there is a hole within the disk region which has no fluid in it (like a bundt cake, or a toroidal pipe) as shown in the right of Fig. 2.6, we cannot use Stoke's theorem and therefore we only know that the circulation is quantized in units of the elementary circulation quantum h/m.

In fact there is no constraint on the size of the hole — the hole in the fluid can be extremely small and this still consitutes a hole in the fluid. We only need a single point where the superfluid density goes to zero such that the phase is no longer defined at that one point. In this case we can have the phase θ wrap by any integer multiple of 2π as we go around this single point. This is known as a "vortex". The existence of vortices in superfluid helium was predicted by Feynmann in 1955[17].

Imagine a bucket of helium above the superfluid transition temperature. We start the bucket rotating so that the circulation is very large

$$\oint \mathbf{v}_S \cdot \mathbf{dl} \gg 0$$

---

[17] As we will discuss below, as similar prediction was made for superconductors somewhat earlier by Abrokosov, but he did not publish it until after Feymann convinced the world that the idea was reasonable.

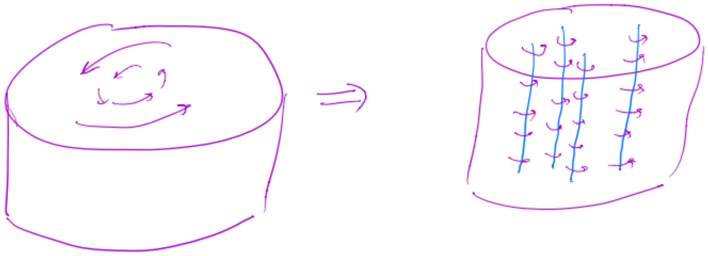

Figure 2.7: If we start a bucket of helium rotating above the critical temperature and then we cool it below the critical temperature, the circulation is accomodated by the introduction of many vortex lines.

We now imagine cooling the system through the transition temperature T_c. Since the superfluid must be curl free, the only way we can accomodate the circulation is to have many point vortices, where there is quantized circulation around each such vortex. Looked at from far away, the velocity flow field is roughly the same in the superfluid phase as it was in the normal phase. As mentioned above, in the core of the vortex (here one dimensional lines) the superfluid density drops to zero. In actual superfluids He, the vortex core is only a few angstrom in diameter.

One often hears arguments that quantized circulation explains the persistant flow phenomenon observed in superfluids. Indeed, one can imagine starting a superfluid flowing around a toroidal pipe. Since the circulation is quantized, it can only decay in discrete steps. If there is some impediment, or activation barrier, to making sudden steps in circulation, one might imagine that this prevents the circulation from decaying at all.

While it is true that the circulation can be locked to a single value, this is actually not sufficient to explain dissipationless flow. The issue is not whether the circulation decays but whether energy is dissipated. Even without having a decay in the circulation (which is the line integral of the *velocity*) one can dissipate energy if some sort of friction heats the fluid. This would slowly reduce the superfluid fraction and increase the normal fraction, thus reducing the superfluid *current*, and eventually the system would have no superfluid left! So the question boils down to whether or not a particular superfluid will dissipate energy. In fact in noninteracting BECs, we will see below that, while circulation is quantized, they do dissipate energy to friction and therefore do not have persistent flow.

2.4 Landau Criterion for Superflow

Landau developed a brilliant argument to determine whether a fluid can flow without dissipating energy.

Let us assume that for a superfluid (and normal fluid) at rest there is some spectrum $\epsilon(\mathbf{p})$ for excitations which we will call "quasiparticles". In a BEC these are simply

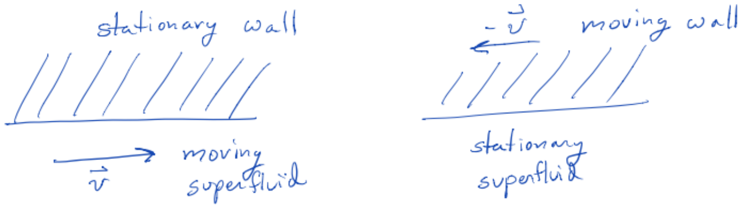

Figure 2.8: Left: Flowing a fluid past a wall. Right: In the fluid frame, the wall is moving.

excitations of particles out of the ground state wavefunction. In an interacting superfluid, these are more complex collective excitations. We need only assume that such excitations exist.

We now imagine flowing the superfluid past a stationary wall at velocity $\mathbf{v}$ as in the right of Fig. 2.8, and we would like to ask whether energy can be dissipated. Another way to ask this is to ask wehether quasiparticles can be excited.

In order to answer this, the argument entirely boils down to figuring out the energy momentum relation *in the rest frame of the superfluid* and then asking whether energy and momentum can be conserved in a process that creates a quasiparticle excitation.

Thus, let us switch to the fluid rest frame as in the right of Fig. 2.8. We know the dispersion $\epsilon_{fluid}(\mathbf{p}) = \epsilon(\mathbf{p})$ of excitations in this (the fluid) frame, and we would like to determine the dispersion relation in the lab frame. A classical Galilean transformation gives us

$$\epsilon_{lab}(\mathbf{p}) = \epsilon_{fluid}(\mathbf{p}) - \mathbf{p} \cdot \mathbf{v} \tag{2.8}$$

Note that here the quantum number $\mathbf{p}$ describes the momentum of the quasiparticle in the fluid frame.

To justify this Galilean transformation (Eq. 2.8) we should recall that in quantum mechanics the phase of the wavefunction oscillates as

$$\psi \sim e^{-i\epsilon t/\hbar}$$

So here we are claiming that a wavefunction for a particle with momentum $\mathbf{p}$ should oscillate as

$$\psi(\mathbf{p}) \sim e^{i\mathbf{p}\cdot\mathbf{x}/\hbar - i\epsilon t/\hbar}$$

If we transform into a moving frame we then have

$$\begin{aligned} \psi(\mathbf{p}) &\rightarrow e^{i\mathbf{p}\cdot(\mathbf{x}+\mathbf{v}t)/\hbar - i\epsilon t/\hbar} \\ &= e^{i\mathbf{p}\cdot\mathbf{x}/\hbar - i(\epsilon - \mathbf{p}\cdot\mathbf{v})t/\hbar} \end{aligned}$$

so we rederive Eq. 2.8.

A more familiar way of understanding this transformation is to think about frequencies $\omega = \epsilon/\hbar$ instead of energies. We then recognize Eq. 2.8 as being the usual Doppler

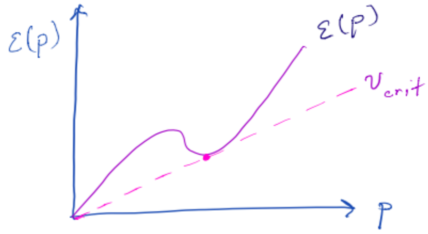

Figure 2.9: A spectrum $\epsilon(p)$ and the corresponding critical velocity for the superfluid.

shift of a frequency in a moving frame[18].

So given Eq. 2.8 our question is whether in the lab frame, the energy to create an excitation is ever negative. If so, excitations are created spontaniously and energy is dissipated. So when does this happen? Obviously $\epsilon - \mathbf{v} \cdot \mathbf{p}$ is minimized when $\mathbf{v}$ and $\mathbf{p}$ are parallel. Thus we can get negative values of ϵ_{lab} only if

$$\frac{\epsilon(p)}{p} < v$$

Given a dispersion $\epsilon(p)$ (in the rest frame), there is thus a critical velocity

$$v_{crit} = \min_p \frac{\epsilon(p)}{p}$$

(see figure 2.9). Below this critical velocity, there is no way to create a quasiparticle while conserving energy and momentum. If the fluid flows at velocity greater than the critical velocity, quasiparticles are spontaneously generated and energy is dissipated from the superflow.

Note now that if one considers a BEC, the spectrum of excitations is simply $\mathbf{p}^2/(2m)$ i.e., just the spectrum of noninteracting particles. The critical velocity is then

$$v_{crit;BEC} = \min_p \frac{p^2/(2m)}{p} = 0 \qquad (!)$$

We thus conclude (as Landau realized intuitively!) that *a noninteracting BEC does not superflow!*

When we add interacting between the bosons, the spectrum develops an acoustic wave (we will see this in more detail later!). In that case we have a low energy spectrum

$$\epsilon(p) = v_{sound}\, p + \ldots$$

---

[18] This argument is strictly correct for situations where the dispersion is linear — i.e., we have sound waves or phonons.

which then gives us a critical velocity

$$v_{crit} = v_{sound}$$

assuming the correction hidden in the "$+ \ldots$" is positive. If it is a negative correction (as shown in Fig. 2.9) the critical velocity can be somewhat lower.

To be a bit more detailed about interacting Bose systems, we recall what we have learned in other courses about the Bogoliubov approach to weakly interacting Bose gases. In fact we will review this technique in section 4.5 below. We derived (and will derive again later in several ways), that for a weakly interacting Bose gas with interaction

$$\frac{U}{2}\sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j)$$

with U being weak, the excitation spectrum is given by

$$\epsilon(p) = \sqrt{(\frac{p^2}{2m} + nU)^2 - (nU)^2}$$

where n is the density of bosons. For small p this can be expanded as

$$\epsilon(p) \sim \frac{p}{\sqrt{2m}}\sqrt{\frac{p^2}{2m} + 2nU}$$

Thus we obtain a crtical velocity

$$\min_p \frac{\epsilon(p)}{p} = \min_p \frac{1}{\sqrt{2m}}\sqrt{\frac{p^2}{2m} + 2nU} = \sqrt{\frac{nU}{m}} = v_{acoustic} = v_{crit}$$

Note: about real experiments

While the Landau theory of critical velocity is quite beautiful and compelling, experiments do not often agree with the Landau estimate. In fact measured critical flow velocities can often be as much as 100 times smaller than the acoustic velocity — and furthermore the critical velocity often depends on the details of the geometry of the experiment.

In thin tubes of superfluid it is easy to qualitatively explain the physics of the critical velocity. This has to do with the physics of vortices and the quantization of circulation. As we mentioned above if we have a toroidal (but thin) tube of fluid, with a fixed circulation going around the tube, this circulation is quantized. This circulation can decay if a vortex is nucleated at one edge of the tube, flows perpendicular to the supefluid flow and then disintegrates at the other edge of the tube. This process can reduce the circulation in discrete steps.

Such a process begins to look much less likely in thick tubes of fluid — however, experiments seem to suggest that vortex physics is still involved.

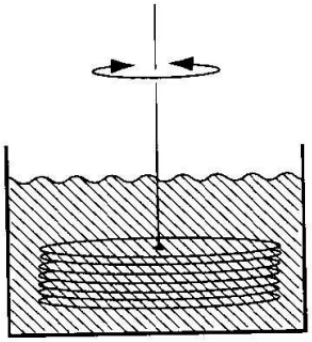

Figure 2.10: The Andronikoshvili experiment. Since normal fluid sticks between the closely spaced disks (but superfluid does not), the moment of inertia of the stack of disks, and hence frequency of oscillation of the disks tells us the fraction of fluid that is superfluid.

2.5 Superfluid Density

Finally we turn to Landau's prediction of the superfluid density as a function of temperature $\rho_S(T)$.

2.5.1 The Andronikoshvili Experiment

Landau made a prediction for the superfluid density $\rho_S(T)$ then convinced a young experimentalist, Elephter Andronikoshvili[19], to make careful measurements of the superfluid density in 1946, and the results supported his predictions (perhaps unsurprisingly since Landau was a genius!).

The experiment is shown in Fig. 2.10. A stack of closely spaced disks is hung in a container of helium by a thin wire which acts as a torsion oscillator. The idea is that when the stack of disks rotates, normal fluid, which is viscous will get stuck between the disks and must rotate with the stack. However superfluid, which has no viscosity slips through the closely spaced disks and does not rotate. The normal fluid thus contributes to the total moment of inertia of the stack, and hence changes the oscillation frequency of the torsion oscillator. By measuring the change in the oscillation frequency as a function of temperature, one can determine the fraction of helium that is superfluid as a function of temperature.

Andronikoshvili clearly measured that the normal fluid density is proportional to T^4

---

[19] In my opinion, this is the coolest name of all physicists. The ending "vili" is Georgian meaning "descendant of". Thus, Elephter was part of a royal Georgian family that traces its ancestery back to Andronikos I of the Eastern Roman Empire in the 1100's. Andronikos seemed quite violent and fittingly met a violent end himself.

at low temperature.

$$\rho_N(T) \sim T^4$$

We should compare this result to a simple calculaton for a noninteracting BEC. We can write the mass of particles that are normal by simply counting the number of particles that are not in the condensate (i.e., not in $\mathbf{p} = 0$). We thus have

$$\rho_N(T) = \frac{m}{V} \sum_{\mathbf{p} \neq 0} n_B(\beta \epsilon(p)) = m \int \frac{d^3p}{(2\pi\hbar)^3} \, \frac{1}{e^{\beta p^2/(2m)} - 1} \tag{2.9}$$

where $\beta = 1/(k_B T)$ as usual, and we have used that

$$n_B(x) = \frac{1}{e^x - 1}$$

is the Bose factor and for the noninteracting Bose particles we have the dispersion $\epsilon(p) = p^2/(2m)$.

We can evaluate Eq. 2.9 by defining $q = \beta^{1/2} p$ giving us

$$\rho_N(T) = m(k_B T)^{3/2} \int \frac{d^3q}{(2\pi\hbar)^3} \, \frac{1}{e^{q^2/(2m)} - 1} \sim T^{3/2} \tag{2.10}$$

which differs markedly from the experimental result!

2.5.2 Landau's Calculation of Superfluid Density

Again this calculation relies on thinking about superfluids in both the lab and the moving superfluid frame as in Fig. 2.8. Here, however, we realize that the normal fluid is dragged by the wall and will have the same velocity as the wall, whereas the superfluid moves seperately (the fluid velocities drawn in Fig. 2.8 are for the super part of the fluid only).

Thus in the frame where the wall is moving but the superfluid is still, the *normal* fluid current (which is the total fluid current) is given by

$$\mathbf{j}_{total} = \mathbf{j}_N = \rho_N \mathbf{v}_N \tag{2.11}$$

and we would like to calculate ρ_N.

As before, in the lab frame we have

$$\epsilon_{lab-frame} = \epsilon(\mathbf{p}) - \mathbf{v} \cdot \mathbf{p}$$

where $\epsilon(\mathbf{p})$ describes the excitation spectrum when the superfluid is in its rest frame. As mentioned in the above section where we calculated critical velocity, if $\epsilon_{lab-frame}$ becomes negative, then we get spontaneous generation of excitations and we get dissipation.

However, even if $\epsilon_{lab-frame}$ is positive, it can still be excited thermally. We expect that the density of such particles will be given by

$$n_B(\beta(\epsilon(\mathbf{p}) - \mathbf{v}\cdot\mathbf{p}))$$

and this gives the occupation probability of the state labeled $\mathbf{p}$ in the superfluid rest frame.

So, in the superfluid rest frame we have the momentum (i.e., the mass current) of the excitations (i.e., of the normal fluid) being given by

$$\mathbf{j}_N = \int \frac{d^3p}{(2\pi\hbar)^3}\ \mathbf{p}\ n_B(\beta(\epsilon(\mathbf{p}) - \mathbf{v}\cdot\mathbf{p}))$$

We can then expand for small $\mathbf{v}$ to obtain

$$\mathbf{j}_N = \int \frac{d^3p}{(2\pi\hbar)^3}\left[\mathbf{p}\ n_B(\beta\epsilon(\mathbf{p})) - \mathbf{p}\beta(\mathbf{v}\cdot\mathbf{p})n'_B(\beta\epsilon(\mathbf{p}))\right]$$

The first term in the brackets vanishes by symmetry. To evaluate the second term, we can assume the velocity $\mathbf{v}$ is in the x direction. We then have

$$j_{N,x} = v_x\beta\int\frac{d^3p}{(2\pi\hbar)^3}p_x^2\left[-n'_B(\beta\epsilon(\mathbf{p}))\right]$$

Referring back to Eq. 2.11 and realizing that the wall velocity v is the normal fluid velocity we obtain the result that

$$\rho_N = \beta\int\frac{d^3p}{(2\pi\hbar)^3}p_x^2\left[-n'_B(\beta\epsilon(\mathbf{p}))\right] \tag{2.12}$$

Case 1: Noninteracting BEC

Let us try plugging in the dispersion $\epsilon(p) = p^2/(2m)$ for a noninteracting BEC. We can scale out the temperature by defining

$$\mathbf{q} = \beta^{1/2}\mathbf{p}$$

to obtain

$$\rho_N = \beta(\beta^{-5/2})\int\frac{d^3q}{(2\pi\hbar)^3}q_x^2\left[-n'_B(q^2/2m)\right] \sim T^{3/2} \tag{2.13}$$

which agrees with our prior calculation of the normal fluid density of a BEC in Eq. 2.10. (With some analytic work it can be shown that the two expressions in fact have the same prefactor too!).

Case 2: Interacting BEC / Superfluid

For an interacting BEC or superfluid, we expect a low energy acoustic mode so that

$$\epsilon(\mathbf{p}) = c|\mathbf{p}| + \ldots$$

Again using Eq. 2.12 we can here instead define $\mathbf{q} = \beta\mathbf{p}$ so that

$$\rho_N = \beta\beta^{-5} \int \frac{d^3q}{(2\pi\hbar)^3} q_x^2 \left[-n_B'(c|q|)\right] \sim T^4 \tag{2.14}$$

in agreement with the results of Andronikoshvili! (Score one more for Landau!)

Heat capacity and a caution

It is correct to write the total internal energy of the Bose system at finite temperature as

$$U = \int \frac{d^3p}{(2\pi\hbar)^3} \, \epsilon(p) n_B(\beta\epsilon(p))$$

Indeed, for a linear (phonon) spectrum this reproduces the usual T^3 Debye heat capacity of phonons at low temperature.

One might wonder whether we could calculate the normal fluid density by just writing

$$\tilde{\rho}_N \sim \int \frac{d^3p}{(2\pi\hbar)^3} \, n_B(\beta\epsilon(p))$$

While this redefinition of the normal fluid density worked in Eq. 2.10 for $\epsilon = p^2/(2m)$ (giving the same result as Eq. 2.13) it generally is not correct! Indeed, for $\epsilon = c|p|$ it fails to give the same result as Eq. 2.14.

The reason is simply that the quantity ρ_N is defined only by Eq. 2.11. One could also define the different quantity $\tilde{\rho}_N$ but this is in fact not a measurable quantity, whereas ρ_N is.

Chapter 3

Charged Superfluid $\approx$ Superconductor

To a large extent the phenomenology of a superconductor can be understood as just being a charged superfluid. This approach (roughly) is known as London theory, invented by Heinz and Fritz London when they were in Oxford in 1935. Historically this was before the discovery of the phenomenon of superfluidity! Indeed, much of the two fluid model was pioneered first in the context of superconductivity.

3.1 London Theory

As with the picture of superfluid Helium, we postulate both a normal and superfluid part of the charged fluid in a superconductor. We will ignore the normal component for now and focus on the motion of the super part — which flows with no dissipation.

A dissipationless fluid will display free acceleration when a force $\mathbf{F}$ is applied. We can thus write

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{\mathbf{F}}{m^*} = \frac{-e^* \mathbf{E}}{m^*}$$

This is essentially Drude theory for a fluid with no scattering. We have written here a charge e^* and a mass m^* of the charge carrier. Note that here only the ratio e^*/m^* enters. This equation does not know whether the charge carrier is a single electron or a pair of electrons or quartets of electrons. However, $e^*/m^* = e/m$ in all cases.

The supercurrent is then written as

$$\mathbf{j}_{super} = -e^* n_S^* \mathbf{v}$$

where n_S^* is the superfluid number density of the charge carriers. We emphasize that this quantity is the *charge density current* rather than the mass density current we discussed when we were discussing Helium superfluid above. Note again that the combination

$-e^* n_S^* = -e n_S$ does not know how big the individual particles are. It could be density n_S of particles of charge $-e$ or could be density $n_S/2$ of particles of charge $2e$ and so forth. The point here is that at level of this London theory, one has no way of knowing that the electrons might pair up into boson clusters.

Putting the last two equations together we derive the so-called First London Equation

$$\frac{\partial \mathbf{j}_{super}}{\partial t} = \frac{(e^*)^2 n_S^*}{m^*}\mathbf{E} \qquad \text{1st London Eq.} \tag{3.1}$$

Again, the charge cluster size here does not matter. Note that this equation is really nothing more than Drude theory with no scattering, and an assumption of a net charge density $-e n_S$.

We can then take the curl of the first London equation and use Faraday's law to replace $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t$ to get

$$\nabla \times \frac{\partial \mathbf{j}_{super}}{\partial t} = \frac{(e^*)^2 n_S^*}{m^*}\nabla \times \mathbf{E} = \frac{-e^2 n_S}{m}\frac{\partial \mathbf{B}}{\partial t}$$

Then integrating both sides $\int dt$ starting at some initial time we get

$$\nabla \times \mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*}\mathbf{B} + \mathbf{C}(\mathbf{r}) \tag{3.2}$$

where $\mathbf{C}(\mathbf{r})$ is independent of time.

We now need to try to figure out what this integration constant $\mathbf{C}$ is. To do so, we imagine starting with a superconductor in $\mathbf{B} = 0$ in its ground state so that $\mathbf{j}_{super} = 0$. In this situation we can take $\mathbf{C}(\mathbf{r}) = \mathbf{0}$ everywhere, at least for this experimental protocol.

Once we have turned on $\mathbf{B}$ we want to consider the possible steady-state solutions. First, we have Ampere's law

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j}_{super} \tag{3.3}$$

Here we are ignoring the normal part of any current, since we are only concerned with current that is persistant. Further, since we are concerned with steady state we will ignore the contribution of $\partial \mathbf{E}/\partial t$. Taking the curl of Amperes' law we get Eq. 3.4. In going from Eq. 3.4 to 3.5 we use a vector identity on the left and Eq. 3.2 on the right. Finally in going to Eq. 3.6 we set $\mathbf{C} = 0$ as suggested above on the right and we use the Maxwell's equation (no monopoles) on the left.

$$\begin{aligned}
\nabla \times (\nabla \times \mathbf{B}) &= \mu_0 (\nabla \times \mathbf{j}_{super}) && (3.4)\\
\nabla(\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} &= \mu_0 \left(\frac{-e^{*2} n_S^*}{m^*}\mathbf{B} + \mathbf{C}(\mathbf{r}) \right) && (3.5)\\
\nabla^2 \mathbf{B} &= \frac{\mu_0 e^{*2} n_S^*}{m^*}\mathbf{B}(\mathbf{r}) && (3.6)
\end{aligned}$$

This last equation has solutions of the form (for example)

$$\mathbf{B}(x) = \mathbf{B}_0 \; e^{\pm x/\lambda} \tag{3.7}$$

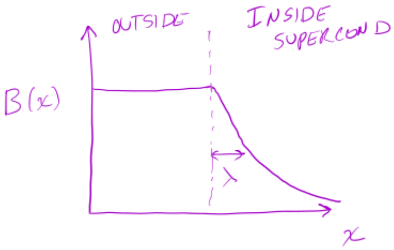

Figure 3.1: Depiction of magentic field decaying exponentially.

where λ is known as the *penetration depth*, and is given by

$$\lambda = \left(\frac{m^*}{\mu_0 n_S^* e^{*2}}\right)^{1/2} \tag{3.8}$$

Once again we emphasize that this quantity does not know the size of the charged particle, but only knows the charge to mass ratio e/m and the total superfluid charge density en_S.

For most superconductors the penetration depth at zero temperature is somewhere between tens and hundreds of nanometers. Note, however, that as T gets very close to the critical temperature from below the superfluid density n_S^* gets very small (and eventually vanishes at T_c as the superfluid fraction goes to zero) so that λ diverges at T_c.

The exponential decay we derived in Eqs. 3.6 and 3.7 is depicted in Fig. 3.1. The magnetic field outside of the superconductor is a constant, but going into the superconductor it decays expontially with a decay length given by λ.

The reason the magnetic field decays going into the superconductor is that the magnetic field is screened by persistant superfluid electric currents. This is similar to Lenz's law: We start with a superconductor in no magnetic field, then we turn on a magentic field and currents flow in the superconductor to prevent the change of the magnetic field and these currents persist indefinitely since there is no resistance to current flow.

However, as we will see next, it turns out that the screening of magnetic field in a superconductor is fundamentally *more* than just Lenz's law!

3.1.1 Meissner-Ochsenfeld Effect

The Meissner-Ochsenfeld Effect (or just "Meissner Effect")[1] demonstrates that the screening of magnetic field from superconductors is not just Lenz's laws.

---

[1] Walther Meissner had established in 1922 one of the world's only helium liquifiers in Berlin. In 1933, Meissner's student, Robert Oschsenfeld discovered that the magnetic field outside fo the superconductor changed when the superconductor is cooled through the critical tempertaure. Meissner got excited by this result and took over the experiment to the large extent.

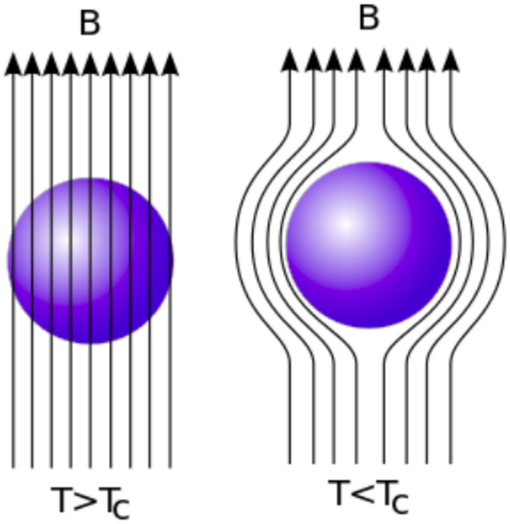

Figure 3.2: The Meissner Effect

To demonstrate the effect, see figure 3.2. On the left we have a material in a magnetic field above its superconducting critical temperture. Then we cool the system down until it becomes a superconductor. While Lenz's law would predict that currents would flow so as to prevent any changes in the magnetic field, what is observed instead is that the magnetic field is completely expelled from the superconductor! So it is not just that the superconductor is a perfect conductor: the superconductor is a perfect diamagnet! The ground state of the total system of superconductor and magnetic field has the magnetic field expelled from the superconductor. Thus the Meissner effect is thermodynamical not dynamical (i.e., Lenz's laws cares about the dynamics of how you get to a situation, the thermodynamic ground state does not).

To explain the Meissner effect the Londons postulated that the integration constant $C(\mathbf{r})$ in Eq. 3.2 is always zero, independent of the initial conditions. Thus we instead write

$$\nabla \times \mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*} \mathbf{B} \qquad \text{2nd London Equation} \tag{3.9}$$

which is known as the Second London equation. We should compare this equation to the curl free condition on superfluid helium, Eq. 2.1. This would be equivalent if we set the charge on the superfluid to zero (set $e^* = 0$) and fix the superfluid density to a constant. .

London Gauge

Both London equations can be summarized with a single equation in terms of the vector potential by writing

$$\mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*} \mathbf{A} \tag{3.10}$$

if we take the curl of this equation, using $\nabla \times \mathbf{A} = \mathbf{B}$ we immediately recover the second London equation Eq. 3.9, whereas if we take the time derivative of this equation, using $\dot{\mathbf{A}} = -\mathbf{E}$ we obtain the first London equation Eq. 3.1. However we note that in order for Eq. 3.10 to make sense we have to work in so-called "London gauge" (or Coulomb Gauge) where

$$\nabla \cdot \mathbf{A} = 0$$

This guarantees that $\nabla \cdot \mathbf{j}_{super} = 0$ which is what we need for a steady state current flow. Further, we must also choose the gauge

$$A_0 = 0$$

so that we have $\mathbf{E} = -\dot{\mathbf{A}}$ (which we already used) rather than $\mathbf{E} = -\dot{\mathbf{A}} - \nabla A_0$ which we would have otherwise.

3.1.2 Quantum Input and Superfluid Order Parameter

At this point we are going to rederive the London equations using input from quantum physics. This particular approach is beyond what the London brothers knew. We have a bit of advantage over the Londons' in that we have most of a century of experience with quantum physics, whereas in the 1930s when they were first introducing these ideas quantum mechanics was quite new[2].

Again let us we write an "order parameter" for the superconductor, which is basically a wavefunction for the superfluid (compare to the discussion of section 2.3). Given such a wavefunction ψ, we can write the condensate current in the usual way we write a current in terms of a wavefunction

$$\mathbf{j} = \frac{e^*}{2m^*}\left[\psi^*(\mathbf{p} - e^*\mathbf{A})\psi - [(\mathbf{p} + e^*\mathbf{A})\psi^*]\psi\right]$$

A few things to note about this equation. First, it is obviously analogous to Eq. 2.5. We have included a prefactor of e^*/m^* because here we are interested in charge current rather than mass current. (Note, as we have mentioned a number of times, this ratio does not know how big the charge carrier is, it just knows the charge-to-mass ratio). Secondly we have minimally coupled the momentum to the vector potential in the usual way charged particles couple to a vector potential.

As in section 2.3 we rewrite the order parameter in terms of a magnitude and a phase[3]

$$\psi(\mathbf{r}) = \sqrt{n_0^*}\, e^{i\theta(\mathbf{r})}$$

---

[2] We have another advantage over the Londons — we are alive and they are dead.

[3] As in the case of superfluid Helium we have the subtlety that strictly speaking the condensate density and the superfluid density do not necessarily match although we think of them as being similar objects. See footnotefoot:N0rho.

Figure 3.3: A superconducting torus. We are considering the path C as drawn.

where here n_S^* is the density of charge carriers in the condensate, so that the total charge density associated with the condensate is[4]

$$\rho_0 = n_0^* e^*.$$

Using $\mathbf{p} = -i\hbar\nabla$ and plugging in this form of ψ into our expresion for the superfluid current we obtain

$$\mathbf{j}_0 = \frac{e^*}{m^*} n_0^* \hbar \nabla\theta - \frac{{e^*}^2 n_0^*}{m^*}\mathbf{A}$$

The first term we identify as being analogous to Eq. 2.6.

We now insert a bit of physical intuition —in the ground state we expect the phase θ of the wavefunction will be a constant. We will prove this later, but for now let us just assume it is true. In this case we immediately recover the London equations in the vector potential form[5] as in Eq. 3.10

$$\mathbf{j}_0 = \frac{-{e^*}^2 n_0^*}{m^*}\mathbf{A} \tag{3.11}$$

3.1.3 Superconducting Vortices

In the case of superfluid helium, we derived vorticity quantization in section 2.3.1 above. Here we would like to do something similar.

Let us consider a thick solid torus of the superconducting substance as shown in Fig. 3.3. We then consider the superconducting current cirulation around the handle of the torus

$$\oint_C \mathbf{j}_{super} \cdot \mathbf{dl} = \frac{e^* n_0^* \hbar}{m^*} \oint_C \nabla\theta \cdot \mathbf{dl} - \frac{{e^*}^2 n_0^*}{m^*} \oint_C \mathbf{A} \cdot \mathbf{dl} \tag{3.12}$$

---

[4] In the previous chapter we used the symbol ρ_0 as total *mass* density. I hope this does not cause confusion!

[5] We have gotten something that seems to make sense only in London gauge. If we choose another gauge we must then not have $\nabla^2\theta \neq 0$ in order to preserve current conservation. This then destroys our intuition of thinking of θ as being similar to the phase in the Helium supefluid where $\nabla^2\theta = 0$.

For the first term on the right, just like in Eq. 2.7, the integral must be 2π times an integer. In the second term on the right, we use Stokes' theorem to give us

$$\oint_{C=\partial D} \mathbf{A}\cdot = \int_D dS \cdot (\nabla \times \mathbf{A}) = \int_D dS \cdot \mathbf{B} = \Phi$$

where here Φ is the magnetic flux enclosed by the path C. Thus Eq. 3.12 can be rewritten as

$$\oint_C \mathbf{j}_{super} \cdot \mathbf{dl} = \frac{e^* n_0^* \hbar}{m^*} 2\pi p - \frac{e^{*2} n_0^*}{m^*} \Phi \tag{3.13}$$

where p is an integer. Rearranging this we have

$$\Phi + \frac{m^*}{e^{*2} n_0^*} \oint_C \mathbf{j}_{super} \cdot \mathbf{dl} = \frac{h}{e^*} p \tag{3.14}$$

The combination on the left hand side is often called the *fluxoid* since it is some modification to the flux. And it is this combination which is quantized. Note also the analogue of this equation to our equation for circulation quantization Eq. 2.7.

If we choose our path C to be deep inside a superconductor, we generally expect the current should be zero (any currents should run mostly on the surface, given the Meissner effect which expells any magnetic field — which currents would produce) in which case we obtain flux quantized in units of a fundamental flux quantum h/e^*.

$$\Phi = \frac{h}{e^*} p \tag{3.15}$$

Note that here it is now crucial that we know how big the charge carrying cluster e^* is! In fact we now know that the "boson" which forms the superconducting superfluid is a charge $2e$ cluster, so we have the elementary superconducting flux quantum given by[6]

$$\Phi_0 = \frac{h}{2e} = 2.067\ldots \times 10^{-15}\,\text{Wb}$$

As with a superfluid, we can take the size of the hole down to zero size. This is known as a superconducting vortex. As with a superfluid, the condensate particle density n_0 must vanish at the center of the vortex and the phase twists around this point[7]. However unlike

---

[6] Quantization of flux through superconducting rings was first observed experimentally in 1961 by Deaver and Fairbank in Stanford and by Doll and Naubauer in Germany. Critical theory support was provided by Nina Byers and C. N. Yang. Yang had recently won a Nobel prize (in 1957) for his prediction of parity breaking in weak nuclear decays. Nina Byers was a fellow of Somerville college Oxford but remained in superposition between Oxford and California for a decade. She eventually converged in California. However, late in life she told me personally that she really had always regretted leaving Oxford. She passed away in 2014.

[7] The prediction of superconducting vortices was first made by Alexei Abrikosov of the Landau School in 1953. However, Landau didn't believe the result and prevented Abrikosov from publishing (Landau was a genius, but he was not always right!). In 1955 Feynman predicted vortices in superfluid Helium and eventually Landau was convinced of the result. Abrikosov's work was published in 1957. He won a Nobel prize for this work in 2003.

superfluid helium the rotation of the fluid is screened by the magnetic field. (Compare the 2nd London Equation, Eq. 3.9 to Eq. 2.1). Thus, the magnetic field penetrates the superconductor within a distance λ of the vortex core and screens the rotation of the fluid. Outside of this region no current flows, and there is no magnetic field.

At whatever distance we draw our path C, we will always have quantized fluxoid. If the path is far away from the vortex core, then there will be no current, and the flux enclosed is quantized. If the path is close to the vortex core, there is very little flux enclosed (let us approximate it as zero) so that the circulation is quantized.

3.1.4 Type I and Type II superconductors

It turns out that there are two types of superconductors, creatively called Type I and Type II. In Type I, magnetic field does not penentrate the superconductor at all – it is completely expelled. This is known as the Meissner phase. Another way of thinking of this is that it is a perfect diamagnet[8] with susceptibility $\chi = -1$, the induced magnetization is exactly enough to precisely cancel the applied magentic field.

If enough magnetic field is applied, the superconductivity is destroyed. At temperature T, the field at which the superconductivity is destroyed is known as $H_c(T)$. This quantity goes to zero at the zero-field critical temperature T_c. (See left of Fig. 3.4) Note that although individual vortices are not stable in type I superconductors, one must still have a quantized magnetic flux through any hole in the superconductor.

The situation is different for type II superconductors. For small enough magnetic fields (below $H_{c1}(T)$, see middle of Fig. 3.4), the magnetic field is completely expelled from the superconductor giving a Meissner phase, similar to type I superconductors. However, for stronger magnetic fields $H_{c1}(T) < H < H_{c2}(T)$ the magnetic field penetrates the superconductor in individual vortex lines. This is known as the vortex phase or Abrikosov phase. (See right of Fig. 3.4). At strong enough fields, above $H_{c2}(T)$, the superconductivity is completley destroyed.

Vortex Pinning

Note that in the vortex phase, if vortices move, then the flux moves with it. This then generates a voltage via the Faraday effect

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} .$$

Thus, in the vortex phase, voltage (and hence resistance) is zero *only* if the vortices are not allowed to move.

The way one arranges for vortices to not move is to have them stick to pieces of disorder. Indeed, there is good reason that vortices stick to disorder. If some disorder

---

[8] To remind you $\mathbf{M} = \chi \mathbf{H}$ defines the susceptibility.

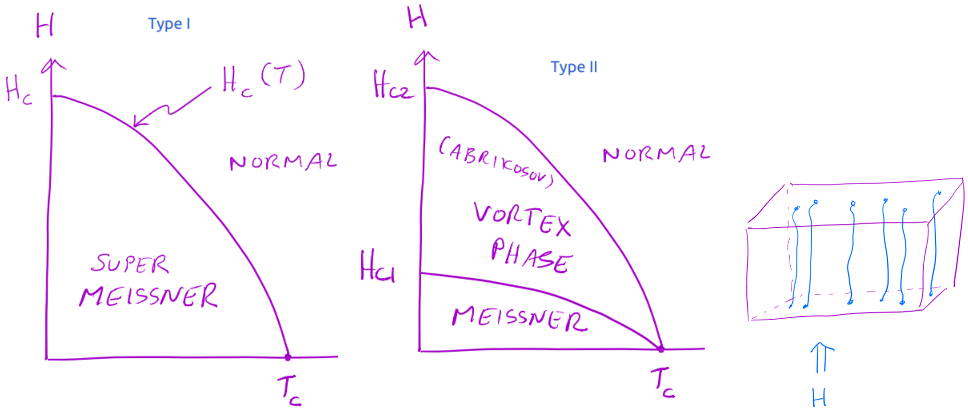

Figure 3.4: The phase diagram of Type I and Type II superconductors. Left: Type I superconductor. Magnetic field is always completely expelled whenever the material is superconducting (i.e, for fields lower than $H_c(T)$. Middle: Type II superconductor. For fields less than $H_{c1}(T)$ the magnetic field is completely expelled. However for fields between $H_{c1}(T)$ and $H_{c2}(T)$, the material is superconducting, and the magnetic field penetrates the material in discrete vortex lines. Right: A depiction of vortices penetrating a sample.

kills superconductivity locally, a vortex that sits at this position costs no energy locally, because there is no superconductivity to kill. Hence vortices will try to stick to regions where superconductivity is already killed.

This phenomenon of vortex pinning being necessary in order to have a true zero resistance state is very similar to our experience with ferromagnets, where domain walls must be pinned by disorder in order to have a true ferromagnet that retains magnetization even in zero field.

3.1.5 How big is H_c

The size of the various critical fields depends on the particular superconductor. Some superconductors have critical fields in the milli-Tesla range, and others have critical fields that are tens of Telsa. Typically the more “robust” superconductors — meaning those with higher critical temperature — also have higher critical fields. Both temperature and magnetic field are perturbations that destroy superconductivity, and it is typically the case that a material that is stongly resistant to one is also strongly resistant to the other.

We can understand the critical fields with more detailed thermodynamics. We start by writing a Gibbs free energy, and consider changing the applied magnetic field $\mathbf{H}$, we have

$$dG = -\mu_0 \mathbf{M} \cdot \mathbf{H} V$$

where V is the volume of the system, and $\mathbf{M}$ is the magnetization (which is magnetic moment per unit volume). For simplicity let us assume that both $\mathbf{H}$ and $\mathbf{M}$ are aligned along the z-axis. We then integrate to obtain

$$G(H,T) - G(H=0,T) = -\mu_0 V \int_0^H dH'\ M(H') \tag{3.16}$$

The magnetization is typically given in terms of a magnetic susceptibility

$$M = \chi H'$$

Let us start by focusing on **type-I superconductors**. Type-I superconductors completely expell the magnetic field, meaning $\chi = -1$ as discussed above. Thus we can substitute into Eq. 3.16 and integrate to obtain

$$G_{super}(H,T) - G_{super}(H=0,T) = \mu_0 V H^2/2 \tag{3.17}$$

whereas for the normal state of a material, typically $\chi \ll 1$ and we have instead

$$G_{normal}(H,T) - G_{normal}(H=0,T) \approx 0$$

Now at the transition into the normal state (H_c) the free energy of the normal state and the free energy of the superconducting state must be the same (hence the transition), so we have

$$G_{super}(H_c,T) = G_{normal}(H_c,T) \approx G_{normal}(0,T)$$

Now substituting into Eq. 3.17 at $H = H_c$ we obtain

$$G_{normal}(H=0,T) - G_{super}(H=0,T) = \mu_0 V H_c^2/2 \tag{3.18}$$

This quantity is known as the *condensation energy*, and it is the amount of energy saved by allowing the material to superconduct rather than remain in the normal state.

On the other hand we can consider the free energy of **type-II superconductors** in a magnetic field. Here, the magnetic field penentrates the superconductor, but guided into flux vortices as shown in the right of Fig. 3.4. We should thus expect that the free energy is given by

$$G_{super}(H) \approx G_{super}(H=0) + N\epsilon L$$

where N is the number of vortices, L is the length of the vortex (i.e., the thickness of the sample) and ϵ is some energy per unit length.

Since each vortex accounts for Φ_0 worth of flux (one flux quantum), we thus have

$$N = \text{number of vortices} = \frac{\text{Area } H\mu_0}{\Phi_0}$$

So that we can write

$$G_{super}(H) = G_{super}(H=0) + \frac{V\epsilon H\mu_0}{\Phi_0}$$

which is linear in magnetic field, compared to Eq. 3.17 for the type I superconductor where the free energy difference is quadratic in magnetic field. We thus obtain a picture

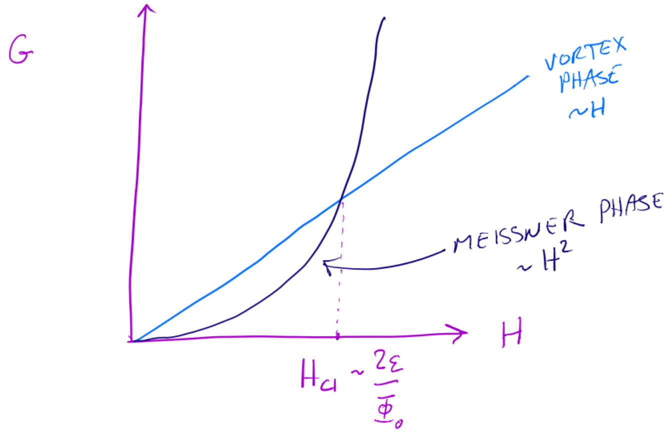

Figure 3.5: Gibbs free energy for the Meissner phase versus the vortex phase. For $H < H_{c1}$ the Meissner phase is the ground state, whereas for $H > H_{c1}$ the vortex phase is lower energy.

like that shown in Fig. 3.5. For applied magnetic fields less than $H_{c1} \approx 2\epsilon/\Phi_0$ the complete expulsion of the magnetic field (i.e., the Meissner phase) is energetically favorable. On the other hand, if $H > H_{c1}$ the vortex phase is lower energy.

Now the actual value of H_{c1} depends on ϵ, the energy per unit length of the vortex line. If ϵ is small, then vortex lines are not energetically costly and correspondingly H_{c1} will be small. If on the other hand, ϵ is large, then H_{c1} will be large. In some cases H_{c1} can be greater than H_c, meaning that the energy per unit length of a vortex is so large that at the magnetic field necessary to force a vortex to penetrate the superconductor, the supercondcutivity is already destroyed. This is precisely the case of a type-I superconductor where there is no vortex phase.

Chapter 4

Microscopic Theory of Bosons

We now try to derive some of the above discussed results on both bosonic superfluids and superconductors using a microscopic quantum mechanical picture.

4.1 Mathematical Preliminaries

We begin with some mathematical preliminaries on using second quantized operators. While many people will have seen this before, it is worth repeating because it is easy to get confused when it comes to some of the more complictated basis transformations and so forth[1].

4.1.1 Second quantization

We start with standard ladder operators for a harmonic oscillator

$$[a, a^\dagger] = 1.$$

The n^{th} mode of the harmonic oscillator, written in normalized form is

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

where $|0\rangle$ is the ground state. The states $|n\rangle$ with $n \geqslant 0$ form an orthonormal set.

The magic of second quantization is that it is entirely equivalent to say that $|n\rangle$ represents n bosons in an orbital!

We can write the number operator, which counts the number of bosons in this orbital as

$$\hat{n} = a^\dagger a = \text{number operator}$$

---

[1] I always get confused as to where the complex conjugations go.

4.1.2 Coherent States

We define a coherent state as

$$\begin{aligned} |\alpha\rangle_c = e^{\alpha a^\dagger}|0\rangle &= \left(1 + \alpha a^\dagger + \frac{\alpha^2 (a^\dagger)^2}{2} + \ldots\right)|0\rangle \\ &= \left(|0\rangle + \alpha|1\rangle + \frac{\alpha^2}{\sqrt{2!}}|2\rangle + \ldots\right) \end{aligned} \tag{4.1}$$

A few comments are in order here. First, we have put a subscript $_c$ on the ket $|\alpha\rangle_c$ to indicate that it is a coherent state. If no confusion will result, we may drop this subscript. Secondly, note that the coherent state $|\alpha\rangle_c$ is not normalized. In fact it is easy to show that[2]

$$_c\langle\alpha|\alpha\rangle_c = e^{|\alpha|^2} \neq 1$$

Similarly the coherent states are not orthogonal

$$_c\langle\alpha|\alpha'\rangle_c = e^{\alpha^*\alpha'}$$

Finally it is worth noting that if we examine the prefactors in Eq. 4.1 which are of the form $\alpha^n/\sqrt{n!}$ we will discover that this combination peaks at roughly $\sqrt{n} \approx |\alpha|$.

The point of using coherent states is that it allows us to turn creation and annihilation operators into numbers as we will now show.

Recall that

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

Applying this to Eq. 4.1 we obtain

$$\begin{aligned} a|\alpha\rangle_c &= \left(0 + \alpha|0\rangle + \frac{\alpha^2}{\sqrt{2!}}\sqrt{2}|1\rangle + \frac{\alpha^3}{\sqrt{3!}}\sqrt{3}|2\rangle + \ldots\right) \\ &= \alpha|\alpha\rangle_c \end{aligned}$$

Thus the coherent state $|\alpha\rangle_c$ is an eigenstate of the annihilation operator with eigenvalue α.

Thus, we can take a and replace it by α if the a operator is acting on the coherent state α. We then get the mapping

$$\begin{aligned} a &\to \alpha & a|\alpha\rangle_c &= \alpha|\alpha\rangle_c \\ a^\dagger &\to \alpha^* & {}_c\langle\alpha|a^\dagger &= {}_c\langle\alpha|\alpha^* \end{aligned}$$

So that a creation operator $a^\dagger$ acting to the left can also be replaced by α^*.

Let us use this principle to do some simple calculation. For example, let us calculate the expectation of the number operator $\hat{n}$ in the coherent state $|\alpha\rangle_c$.

---

[2] It is a simple excercise to show these! Try it!

We have (recalling that are working with non-normalized states)

$$\langle \hat{n} \rangle = \frac{{}_c\langle \alpha | a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c}$$

Allowing the a to act to the right and the $a^\dagger$ to act to the left we obtain

$$\langle \hat{n} \rangle = \frac{|\alpha|^2 \; {}_c\langle \alpha | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = |\alpha|^2$$

Let us next try to calculate $\langle \hat{n}^2 \rangle$. Similarly we get

$$\langle \hat{n}^2 \rangle = \frac{{}_c\langle \alpha | a^\dagger a \, a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = \frac{{}_c\langle \alpha | a^\dagger a^\dagger a \, a + a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = |\alpha|^4 + |\alpha|^2$$

where we have used commutations to put the operators into normal order (all creation operators at the far left).

Using these two results we calcuate the variance of the number of bosons in the coherent state

$$\mathrm{Var}_N = \sqrt{\sigma_N^2} = \sqrt{\langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2} = \sqrt{|\alpha|^2} = \sqrt{\langle \hat{n} \rangle}$$

The important result here is that for large $\langle \hat{n} \rangle$ the fluctuations in particle number are much smaller than the mean – so it won't matter if we fix the particle number or we allow it to fluctuate. Given that the fluctuations are small, a system with a fixed particle number is not very different from a coherent state.

A comment for those who have not explored coherent states before: Laser light can be thought of as a coherent state of photon (which are, appropriately, bosons).

Number-Phase Relation

An interesting feature of coherent states (which will also be true of superfluids) is that number and phase form a quantum mechanical conjugate pair, like momentum and position — you cannot know both at the same time. To see this, let us write the parameter $\alpha = |\alpha| e^{i\varphi}$, we then have

$$|\alpha\rangle_c = e^{|\alpha| e^{i\varphi} a^\dagger} |0\rangle = \left(|0\rangle + |\alpha| e^{i\varphi} |1\rangle + \frac{|\alpha|^2 e^{2i\varphi}}{\sqrt{2!}} |2\rangle + \ldots \right)$$

Now let us try differentiating with respect to the phase

$$-i \frac{\partial}{\partial \varphi} |\alpha\rangle_c = \left(0|0\rangle + 1|\alpha| e^{i\varphi} |1\rangle + 2 \frac{|\alpha|^2 e^{2i\varphi}}{\sqrt{2!}} |2\rangle + \ldots \right)$$

which we realize is exactly the same as applying the number operator to the coherent state (i.e., it multiplies $|n\rangle$ by n). Thus we identify

$$-i \frac{\partial}{\partial \varphi} = \hat{n} \tag{4.2}$$

analogous to $-i\hbar\partial/\partial x = \hat{p}$. Thus we expect if we are going to have a superfluid with a well defined phase we must also accept that it will have an indefinite number of particles. We will see this in detail below.

4.1.3 Multiple orbitals

Let us now consider the case of bosons which are allowed to reside in multiple orbitals. Let us assume we have an orthonormal set of orbitals which we will label $i, j, \ldots$. For each orbital i we have a corresponding creation operator $a_i^\dagger$ and annihilation operator a_i. These operators obey the commutations

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{4.3}$$

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \tag{4.4}$$

In other words, the creation and annhilation operators in a given orbital are completely independent from the creation and annihilation operators from another orbital.

We also define a ket $|0\rangle$ to mean the vacuum of all the orbital; i.e., no bosons at all. Thus $a_1^\dagger|0\rangle$ means one boson in orbital 1, whereas $a_1^\dagger \frac{(a_2^\dagger)^2}{2!}|0\rangle$ means two bosons in orbital 2 and one boson in orbital 1, and so forth.

It is crucial that we are able to change basis for our orbitals. Suppose we have two seperate complete sets of orthonormal bases. Let us call the first set $\{|\phi_n\rangle\}$ and call the second set $\{\psi_m\}$. As an example we might imagine that one set is a set of plane waves, whereas maybe the other set is a set of harmonic oscillator wavefunctions. The conversion between the two corresponding sets of creation operators is given by

$$a^\dagger_{\phi_n} = \sum_m \langle \psi_m | \phi_n \rangle \, a^\dagger_{\psi_m} \tag{4.5}$$

A very importnat example is the case of particles hopping on a lattice. Here we have a natural tight binding basis where $\psi_{\mathbf{r_0}}(\mathbf{r}) = \delta_{\mathbf{r},\mathbf{r_0}}$ is a wavefunction of a particle localized at position $\mathbf{r}$ and the corresponding second quantized operator that creates a particle in this orbital is $a^\dagger_{\mathbf{r}}$. On the other hand, we also have the plane wave orbitals

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

with N the number of sites in the system. We write the corresponding second quantized operators that create a particle in these plane waves as

$$a^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} a^\dagger_{\mathbf{r}} \tag{4.6}$$

Any operator can be written in second quantized notation in any basis — this is done by representing it in terms of its matrix elements in that basis. For example, a one-body operator can be written as

$$\hat{O} = \sum_{n,m} \langle n|\hat{O}|m\rangle a_n^\dagger a_m$$

Similarly one can write a two body operator as

$$\hat{O} = \sum_{n,m,q,p} (\langle n| \otimes \langle q|)\ \hat{O}\ (|m\rangle \otimes |p\rangle)$$

and so forth.

Continuum Limit

Very frequently we take the continuum limit where $\mathbf{r}$ lives not on a lattice, but in a continuum. In this case we conventionally replace the creation and annhilation operators $a_{\mathbf{r}}^\dagger$ and $a_{\mathbf{r}}$ with the continuum field operator $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$. The corresponding commutation relations are then given by

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

In terms of these field operators the plane wave creation operators are given by

$$a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{V}} \int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}\, \hat{\psi}^\dagger(\mathbf{r})$$

with V the volume of the system.

Indeed, any orbital basis $\{\phi_n\}$ can be written in terms of the continuum field operators as

$$a_{\phi_n}^\dagger = \int d\mathbf{r}\, \phi_n(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})$$

The transformation in reverse, assuming we are working with a complete basis, is given by

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{r}) &= \sum_n \langle \phi_n|\mathbf{r}\rangle a_{\phi_n}^\dagger \\ &= \sum_n \phi_n^*(\mathbf{r}) a_{\phi_n}^\dagger \end{aligned} \tag{4.7}$$

4.2 BECs and the Gross-Pitaevskii Equation

We will now use second quantized operators to examine some of the physics of BECs and interacting bosons. We begin by considering noninteracting bosons.

4.2.1 Noninteracting BECs as Coherent States

The principle of a BEC is that we want to put many bosons in the same oribtal. Let us call this orbital ϕ_0, and write a creation operator $a^\dagger_{\phi_0}$ that creates a boson in this orbital. Now let us write a coherent state for many bosons in this orbital.

$$|\alpha; \phi_0\rangle \equiv e^{\alpha a^\dagger_{\phi_0}} |0\rangle$$

Enirely analogous to our above calculation we can calculate the expectatoin of the number of bosons in this orbital

$$\langle N_0 \rangle = \frac{\langle \alpha; \phi_0 | a^\dagger_{\phi_0} a_{\phi_0} | \alpha; \phi_0 \rangle}{\langle \alpha; \phi_0 | \alpha; \phi_0 \rangle} = |\alpha|^2$$

meaning that the coherent state puts (on average) $|\alpha|^2$ bosons into the orbital ϕ_0.

It is very useful to examine the effect of the field operator $\hat{\psi}(\mathbf{r})$ on the coherent state. To do this we use the decomposition given in Eq. 4.7 to give

$$\begin{aligned} \hat{\psi}(\mathbf{r}) |\alpha; \phi_0\rangle &= \sum_n \phi_n(\mathbf{r}) a_{\phi_n} |\alpha; \phi_0\rangle && (4.8) \\ &= \alpha \phi_0(\mathbf{r}) |\alpha; \phi_0\rangle && (4.9) \end{aligned}$$

Thus, using a coherent state turns the field operator $\hat{\psi}(\mathbf{r})$ into a scalar

$$\hat{\psi}(\mathbf{r}) \to \psi(\mathbf{r}) = \alpha \phi_0(\mathbf{r}) = \sqrt{N_0}\ \phi_0(\mathbf{r})$$

where we assume the phase of α is real in the last step (although we did not have to make this assumption). Thus the field operator becomes $\psi(\mathbf{r})$ which is simply the ground state wavefunction ϕ_0 normalized to have N_0 particles.

4.3 Interacting Bosons and the Gross-Pitaevskii Equation

We now turn to consider interacting bosons. We write a first quantized Hamiltonian as

$$H = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i - \mathbf{r}_j) \qquad (4.10)$$

Here, the term in bracket is a single paricle Hamiltonian, and we have included possibly a trapping potential $V(\mathbf{r})$. We can also include a chemical potential inside of V if we wish. The final term in the Hamiltonian is some intaction between the bosons.

We can now convert the first quantized Hamiltonian to second quantized form. This is a straightforward exercise[3] yielding

$$\begin{aligned} H &= \int d\mathbf{r}\; \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) \\ &+ \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' : \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\; U(\mathbf{r}-\mathbf{r}')\; \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}') : \end{aligned}$$

In the second line we have the density $\rho(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$ so that this term is an interaction between density at position $\mathbf{r}$ and position $\mathbf{r}'$. We have also included :'s around this term to indicate that the term should be interpreted as being normal ordered — i.e., all creation operators moved to the left. It is clear that this is necessary since applying this term to a state with a single boson should give a zero interaction energy (and this will not be the case unless the term is normal ordered)[4].

From here we will further specialize to a particularly simple delta-function interaction

$$U(\mathbf{r}-\mathbf{r}') = U\,\delta(\mathbf{r}-\mathbf{r}') \tag{4.11}$$

with U a scalar. Such a short range interaction is actually a very good respresentation of the interaction for many physical bosonic systems. For example, for superfluid helium, the Helium atoms are strongly repulsive only at very short distance, and so this is actually a fairly good approximation. Similarly for modern cold-atom BECs, it is often the case that the delta function interaction is actually very representative of the physical system.

This then simplifies our Hamiltonian to the form

$$H = \int d\mathbf{r}\; \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{U}{2}\int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{4.12}$$

Let us now consider a coherent state in an orbtial $\phi(\mathbf{r})$ as a trial wavefunction.

$$|\alpha;\phi\rangle = e^{\alpha a^\dagger_\phi}|0\rangle$$

As discussed above, application of the field operator $\hat{\psi}(\mathbf{r})$ to this coherent state generates the number $\psi(\mathbf{r}) = \alpha\phi(\mathbf{r})$ with $|\alpha| = \sqrt{N}$.

We now calculate the expectation of the Hamiltonian in this coherent state

$$\begin{aligned} \langle H \rangle &= \frac{\langle\alpha;\phi|H|\alpha;\phi\rangle}{\langle\alpha;\phi|\alpha;\phi\rangle} \\ &= \int d\mathbf{r} \left(\psi^*(\mathbf{r}) \left[\frac{-\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \psi(\mathbf{r}) + \frac{U}{2}|\psi(\mathbf{r})|^4 \right) \end{aligned}$$

---

[3] Try it! The trick is to convert terms to a convenient basis — position space or momentum space — as necessary.

[4] Note that leaving the term un-normal ordered will only make an order 1 error in an order N term, so for large numbers of particles it is not a bad mistake!

Finally integrating by parts to handle the derivative we get

$$\langle H \rangle \;=\; \int d\mathbf{r} \left(\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{U}{2} |\psi(\mathbf{r})|^4 \right)$$

This expression is known as the Gross-Pitaevskii (or Ginzburg-Landau) form. This was first discussed by Vitali Ginzburg and Landau in 1950 in the context of superconductivity[5]. In 1960 it was rederived by both Gross (in the west) and Pitaevskii (in the USSR) in the context of superfluid Helium.

Minimizing the energy by taking a functional derivative and setting it to zero,

$$\frac{\delta \langle H \rangle}{\delta \psi^*(\mathbf{r})} = 0$$

we obtain

$$\left[\frac{-\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + U |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = 0 \tag{4.13}$$

which is known as the Gross-Pitaevskii equation, or non-linear-Schroedinger equation. We will study the solutions to this equation later. This simply the single particle Schroedinger equation where there is an additional potential $U|\psi(\mathbf{r})|^2$ making the local potential higher in regions where there are many bosons (the energy eigenvalue can be absorbed into V).

4.3.1 Rederivation without Coherent States

Is there an easier way to get to the Gross-Pitaevskii equation? Do we need to work in a "grand-canonical ensemble" where the number of bosons is indefinite? Do we really have to work with second quantized operators?

The answer to these questions are: Yes, there is an easier way. We don't need any of these technical tools. In fact we can work with first quantized operators with a fixed number of particles.

Recall that a BEC wavefunction puts a macroscopic number of particles in a single orbital $\phi(\mathbf{r})$. So let us write a trial wavefunction for such a BEC as follows:

$$\Psi = \prod_{i=1}^{N} \phi(\mathbf{r}_i)$$

Note that this wavefunction is properly antisymmetic under exchange of particle positions as a bosonic wavefunction should be.

We then find the expectation of our first quantized Hamiltonian Eq. 4.10 for our trial state

$$\langle \Psi | H | \Psi \rangle = N \int d\mathbf{r} \; \phi^*(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \phi(\mathbf{r}) + \frac{N(N-1)}{2} \int d\mathbf{r} \int d\mathbf{r}' : |\phi(\mathbf{r})|^2 \; U(\mathbf{r} - \mathbf{r}') \; |\phi(\mathbf{r}')|^2$$

---

[5] Ginzburg won a Nobel prize for this work in 2003. It is worth reading Ginzburg's Nobel biography. It seems his early years, growing up in the Stalinist Soviet Union were somewhat harrowing!

making the substitution $\psi = \sqrt{N}\phi$ and neglecting the distinction between N and $N-1$ we get exactly the same result as when we used coherent states above. Minimizing the total energy in either approach will allow us to calculate the best single orbital $\phi(\mathbf{r})$, or equivalently ψ, which we should macroscopically occupy to form a BEC.

4.4 Order Parameter and Off-Diagonal Long Ranged Order

So if it is possible to derive everything with such a simple first quantized approach, why then did we go through the extra work of working with coherent states and using second quantization? The reason is that for an interacting BEC (particularly a strongly interacting BEC) it is in fact *not* correct to put all the bosons in a single orbital. A single orbital may be multipy occupied, but due to the interactions some bosons will be kicked out of this single orbital. We will discuss this physics in more detail later. However, despite this complication

$$\langle \hat{\psi}(\mathbf{r}) \rangle \tag{4.14}$$

will remain a good order parameter and a good description, and a convenient description, of the condensate.

It is worth noting, however, that there are some who object to the use of such an object as an order paramter. The obvious objection is that it is perfectly possible to consider a system of bosons with a fixed number, in which case the order parameter Eq. 4.14 is strictly zero and one needs to think a bit harder[6]. It is enlightening to go through some extra work to try to understand in a bit more detail the physics of the superfluid order parameter for the case of fixed particle number.

Let us try to be a bit more precise with our definition of the order paramter for a system with strongly interacting bosons. We can here work with a fixed number of particles (a canonical ensemble). Let us write the folowing density operator

$$\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle \tag{4.15}$$

This operator removes a particle from position $\mathbf{r}$ and puts a particle back in at position $\mathbf{r}'$. While this conserves total particle number, it does not *locally* conserve particle number if $\mathbf{r}$ and $\mathbf{r}'$ are very different. In terms of the multi-particle wavefunction, this object can be written as

$$\rho_1(\mathbf{r}', \mathbf{r}) = N \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \Psi^*(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N) \Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N) \tag{4.16}$$

We can even write this quantity at finite temperature more generally as

$$\rho_1(\mathbf{r}', \mathbf{r}) = \frac{N}{Z} \sum_n e^{-\beta E_n} \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \Psi_n^*(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N) \Psi_n(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

---

[6] The Nobel Laureate Tony Leggett in particular has emphasized the shortcomings of a number non-conserving order parameter

where here E_n and Ψ_n are the n^{th} eigenenergy and eigenvector of the system and $Z = \sum_n e^{-\beta E_n}$ the partition function.

Note also that $\rho_1(\mathbf{r}, \mathbf{r})$ is just the regular density at position $\mathbf{r}$, and if we wanted to, we could write even more complicated operators such as

$$\rho_2(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2)$$

which would be an analogous expression with $N - 2$ integrals.

For a moment, let us think of positions $\mathbf{r}'$ and $\mathbf{r}$ as being discrete. In this case, we can think of $\rho_1(\mathbf{r}', \mathbf{r})$ as actually being a matrix (it has two indices, $\mathbf{r}'$ and $\mathbf{r}$). Since this matrix is hermitian it can be diagonalized and written in terms of its eigenvalues, which we call N_α and its eigenvectors which we call $\phi_\alpha(\mathbf{r})$. We thus have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \sum_\alpha N_\alpha \, \phi^*_\alpha(\mathbf{r}')\phi_\alpha(\mathbf{r}) \tag{4.17}$$

where the eigenvectors are normalized

$$\int d\mathbf{r} |\phi_\alpha(\mathbf{r})|^2 = 1$$

By convention we order the eigenvalues so that N_0 is the largest.

Noninteracting BEC at $T = 0$

For a noninteracting BEC at zero temperature, all of the bosons are in the same orbital. In this case it is easy to calculate that there is only one nonzero eigenvalue $N_0 = N$, the number of particles in the system, and ϕ_0 is the single macroscopically occupied orbital.

Let us consider this case in a bit more detail. For a noninteracting BEC without a trapping potential at $T = 0$, all of the bosons are in the single $\mathbf{k} = 0$ eigenstate, $\phi_0 = 1/\sqrt{V}$. We can then explicitly calculate the order parameter. The easiest way to calculate this is to go back to second quantized form of Eq. 4.15. We then have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle = N\phi^*_0(\mathbf{r}')\phi_0(\mathbf{r}) = N/V$$

the particle density, for all $\mathbf{r}$ and $\mathbf{r}'$. See also the more detailed calculation in section 4.4.1 below.

More generally

However, we expect that even for a BEC for $0 < T < T_c$, there should be a single eigenvalue N_0 which will be smaller than N but still extensively large (we will demonstrate this below). Further, even for an interacting system, we can use N_0 being extensive as an indication of the existance of a condensate and ϕ_0 is the condensate wavefunction. Putting these two together into an order parameters, we have

$$\psi(\mathbf{r}) = \sqrt{N_0}\, \phi_0(\mathbf{r})$$

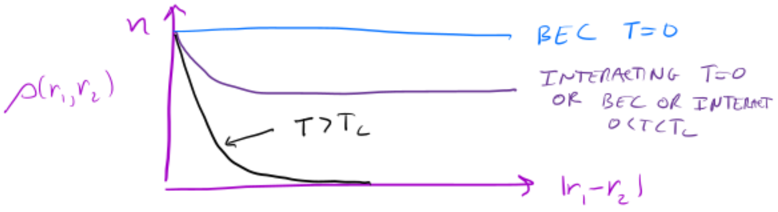

Figure 4.1: Measure of Off-Diagonal Long Range Order $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$. For $\mathbf{r}_1 = \mathbf{r}_2$ we always have $\rho_1 = n = N/V$ the density. However, for $\mathbf{r}_1$ far from $\mathbf{r}_2$ a nonzero ρ_1 indicates the presence of a condensate. For a noninteracting BEC at $T = 0$ (top line) $\rho_1 = n$ for all $|\mathbf{r}_1 - \mathbf{r}_2|$. For a system in the normal phase, $T > T_c$, we have ρ_1 decaying to zero for large $|\mathbf{r}_1 - \mathbf{r}_2|$ as shown in the bottom line. The middle line shows that for a noninteracting BEC at $0 < T < T_c$ or for an interacting BEC at any $T < T_c$, then ρ_1 decays to a constant less than n but larger than zero.

We can make a plot of ρ_1 for severeal different cases as shown in Fig. 4.1.

Recall that $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$ is always just the density n for $\mathbf{r}_1 = \mathbf{r}_2$.

As shown in the figure (and we just discussed) for a noninteracting BEC at $T = 0$ we have $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$ is constant as a function of distance $|\mathbf{r}_1 - \mathbf{r}_2|$. For a normal system without a condensate $T > T_c$, we have ρ_1 decaying to zero for large $|\mathbf{r}_1 - \mathbf{r}_2|$. We will prove this explicitly below.

Another case shown in the figure, that we will derive below is the case of a noninteracting BEC for $0 < T < T_c$. In this case ρ_1 decays to a constant larger than zero, but less than n for large $|\mathbf{r}_1 - \mathbf{r}_2|$.

More difficult to show, however, is the case of an *interacting* Bose system below its critical temperature (possibly at $T = 0$, but possibly at $0 < T < T_c$). The behavior here is similar to that of a BEC at $0 < T < T_c$, that is ρ_1 decays to a constant larger than zero, but less than n for large $|\mathbf{r}_1 - \mathbf{r}_2|$. Qualitiatively this is again due to the fact that, similar to temperature, the interactions "kick" some of the bosons out of the single condensed state. For example, for superfluid Helium at $T = 0$ at large $|\mathbf{r}_1 - \mathbf{r}_2|$ the value of ρ_1 is less than 10% of the density.

The fact that the ρ_1 correlator becomes a constant for large $|\mathbf{r}_1 - \mathbf{r}_2|$ in the superfluid phase is known as *Off-Diagonal Long Ranged Order*[7]. It is sometimes abbreviated as ODLRO. The reason it is called 'off-diagonal" comes again from thinking about ρ_1 as a matrix with two indices, $\mathbf{r}_1$ and $\mathbf{r}_2$ which are taken different from each other (hence off-diagonal). The idea of using this quantity as an indicator of superfluid order is due to

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[7] In comparison, *diagonal long range order* would be long range order in $\rho(\mathbf{r}, \mathbf{r})$ or the density — such as crystalization.

Oliver Penrose[8] in 1951 and the Nobel Laureate Lars Onsager in 1956.

4.4.1 non-interacting bosons at $T \geqslant 0$

It is easy enough to calculate ρ_1 explicitly for a noninteracting Bose system at finite temperature (we will again assume no trapping potential so the single particle eigenstates are plane waves). It is again easiest to work with the second quantized definition of ρ_1 given in Eq. 4.15. We can also decompose the field operator into Fourier modes

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.18}$$

We thus have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle = \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} \langle a^\dagger_{\mathbf{k}'} a_{\mathbf{k}}\rangle e^{i\mathbf{k}\cdot\mathbf{r} - i\mathbf{k}'\cdot\mathbf{r}'} = \frac{1}{V}\sum_{\mathbf{k}} \langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \tag{4.19}$$

Where we can always write

$$\langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle = n_B(\epsilon_{\mathbf{k}})$$

where $\epsilon_{\mathbf{k}}$ is the energy of the boson in mode $\mathbf{k}$ and n_B is the Bose factor.

Thus we have explicitly

$$\rho_1(\mathbf{r}', \mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}} n_B(\epsilon_{\mathbf{k}}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

Now for $T > T_c$ we have n_B being a smooth function of $\mathbf{k}$. We can then freely convert the sum into an integral, and get the usual Fourier transform. Since we are Fourier transforming a smooth function the result ρ_1 is smooth and goes to zero for large $(\mathbf{r} - \mathbf{r}')$.

However, for $T < T_c$ we cannot convert the sum into an integral since a macroscopic number of particles are in the $k = 0$ state. In this case we need to separate $k = 0$ from the sum over $\mathbf{k}$, and then the remainder can be considered a smooth integral.

We then have instead

$$\langle a^\dagger_0 a_0\rangle = N_0(T)$$

and correspondingly

$$\rho_1(\mathbf{r}', \mathbf{r}) = \frac{N_0}{V} + \frac{1}{V}\sum_{\mathbf{k}\neq 0} n_B(\epsilon_{\mathbf{k}}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

where the sum is again a smooth and decaying function.

---

[8] Brother of Roger Penrose.

4.4.2 Current and the Order Parameter

Several times we have treated the order parameter for the condensate as if it is a wavefunction and blithely written things like (See for example, Eq. 2.5)

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2}\left(\psi^* \mathbf{p}\, \psi - (\mathbf{p}\psi^*)\, \psi\right)$$

Is this really legitimate? Indeed, we can essentially derive this equation from the definition of the order parameter as ODLRO.

Let us first write a general expression for the total mass current

$$\mathbf{J} = \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \frac{1}{2}\left(\Psi^* \mathbf{P} \Psi - (\mathbf{P}\Psi^*))\Psi\right)$$

where

$$\Psi = \Psi(\mathbf{r}_1, \ldots \mathbf{r}_N)$$

is the many-body boson wavefunction, and

$$\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$$

is the total momentum.

We realize that since the wavefunction is fully symmetric under interchange between particles we can write

$$\mathbf{J} = N \int d\mathbf{r}_1 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \frac{1}{2}\left(\Psi^* \mathbf{p}_1 \Psi - (\mathbf{p}_1\Psi^*))\Psi\right)$$

Further we can write the *local* mass current density as

$$\mathbf{j}(\mathbf{r}) = N \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \frac{1}{2}\left(\Psi^* \mathbf{p}_1 \Psi - (\mathbf{p}_1\Psi^*))\Psi\right)_{\mathbf{r}_1=\mathbf{r}}$$

This expression is entirely general and applies to any bosonic system. Since $\mathbf{p}_1 = -i\hbar\nabla$ this can be rewritten as

$$\mathbf{j}(\mathbf{r}) = \frac{-i\hbar N}{2} \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \left(\Psi^* \nabla_1 \Psi - (\nabla_1\Psi^*))\Psi\right)_{\mathbf{r}_1=\mathbf{r}}$$

Then writing

$$\begin{aligned}
& \left[\Psi^* \nabla_1 \Psi - (\nabla_1 \Psi^*))\Psi\right]_{\mathbf{r}_1=\mathbf{r}} \\
& = \left[\Psi^*(\mathbf{r}_1', \mathbf{r}_2, \ldots \mathbf{r}_N)\nabla_1 \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N) - (\nabla_{1'}\Psi^*(\mathbf{r}_1', \mathbf{r}_2, \ldots \mathbf{r}_N)))\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)\right]_{\mathbf{r}_1=\mathbf{r}_1'=\mathbf{r}} \\
= \;\; & [\nabla_1 - \nabla_{1'}] \;\; \Psi^*(\mathbf{r}_1', \mathbf{r}_2, \ldots \mathbf{r}_N)\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)\Big|_{\mathbf{r}_1=\mathbf{r}_1'=\mathbf{r}}
\end{aligned}$$

Comparing to the definition of the one-body density matrix in Eq. 4.16 the current density is thus written as

$$\mathbf{j}(\mathbf{r}) = \frac{-i\hbar}{2}\left[\nabla_1 - \nabla_{1'}\right] \rho_1(\mathbf{r'}_1, \mathbf{r}_1)\big|_{\mathbf{r}_1=\mathbf{r}'_1=\mathbf{r}} \qquad (4.20)$$

Now recall the decomposition of the density matrix in terms of its eigenvalues and eigenvectors as in Eq. 4.17, where we have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \psi^*(\mathbf{r}')\psi(\mathbf{r}) + \ldots \qquad (4.21)$$

where $\psi = \sqrt{N_0}\,\phi_0$ is the order parameter of the condensate, and the ... represents many additional terms where the eigenvalues are small — -terms that do not represent the condensate.

Using Eq. 4.21 in Eq. 4.20 immediately recovers

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2}\left(\psi^* \mathbf{p}\, \psi - (\mathbf{p}\psi^*)\, \psi\right) + \ldots$$

o where the ... are the contributions from the noncondensate part of the system.

4.5 Bogoliubov Theory for the Weakly Interacting Bose Gas

Above we mentioned that we would analyze the effect in more detai. We claimed that the interactions somehow "kick" bosons out of the condensate leaving $\rho_1(\mathbf{r}, \mathbf{r}')$ at long distance (large $\mathbf{r} - \mathbf{r}'$) less than the full physical density even at zero temperate.

The approach we follow here, so-called Bogoliubov Theory[9] is a controlled approximation accurate in the limit of weak, but non-zero interaction.

For simplicity let us consider the case where there is no external trapping potential $V(\mathbf{r}) = 0$ so that the single particle eigenstates are plane waves. We will further, for simplicity, assume the inter-particle interaction is a delta function as in Eq. 4.11. Neither of these assumptions is required for the method to work, although both make the calculation easier.

The Hamiltonian in second quantized form, as in Eq. 4.12 is given by

$$H = \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\left[\frac{-\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right]\hat{\psi}(\mathbf{r}) + \frac{U}{2}\int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})$$

Since the single particle eigenstaetes are plane waves we can conveniently write the field operator $\hat{\psi}(\mathbf{r})$ in Fourier modes

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad (4.22)$$

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[9] Nikolay Bogoliubov is probably more famous as a mathematician than a physicist. Nonetheless he also had several important contributions to the physics world, including being one of the B's in BBGKY from statistical physics.

and rewrite the Hamiltonian in the form

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{U}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4} \; \delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4} \tag{4.23}$$

Now we expect that even when we turn on the interactions, the $\mathbf{k} = \mathbf{0}$ mode should be macroscopically occupied at zero temperateure as it is in a BEC. However the commutator

$$[a^\dagger_{\mathbf{0}} a_{\mathbf{0}}, \text{Interaction}] \neq 0$$

which means that the interaction must kick some of the particles out of the $\mathbf{k} = \mathbf{0}$ state. Nonetheless, we still expect macroscopic occupancy of this orbital. Let us thus assume that the $\mathbf{k} = \mathbf{0}$ orbital is in a coherent state with mean occupancy N_0 with $1 \ll N_0 < N$. At $T = 0$ if the interaction were zero, then $N_0 = N$. For sufficiently weak interaction, we might expect that

$$N - N_0 \ll N$$

Post-facto, we will verify that this is true for weak interaction.

Since we have a coherent state, as usual this allows us to replace operators $a^\dagger_{\mathbf{0}}$ and $a_{\mathbf{0}}$ with numbers via the usual substitution

$$a^\dagger_{\mathbf{0}} \to \sqrt{N_0} \qquad\qquad a_{\mathbf{0}} \to \sqrt{N_0}$$

Returning to our Hamiltonian, we now have a small parameter $1/N_0$ and we can organize the parts of the Hamiltonian Eq. 4.23 in terms of which has the most factors of N_0 (i.e., the most factors of $a^\dagger_{\mathbf{0}}$ or $a_{\mathbf{0}}$). In fact, the kinetic term has no factors of N_0 (since the kinetic energy of the $\mathbf{k} = \mathbf{0}$ state is zero). We thus turn to the interaction term and try to organize the pieces of the sum in order of which pieces have the most factors of N_0.

Looking at the sum over $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$, the single term where

$$\mathbf{k}_1 = \mathbf{k}_2 = \mathbf{k}_3 = \mathbf{k}_4 = 0$$

is the largest term, giving us four factors of $\sqrt{N_0}$ Thus the value of this term in the sum is simply the constant

$$\frac{U}{2V} N_0^2 \tag{4.24}$$

At next order We look for a term where there are three factors of $\sqrt{N_0}$ meaning three of the $\mathbf{k}$'s are zero and one is nonzero. However, the delta function in the interaction term of Eq. 4.23 requires that if three of the $\mathbf{k}$'s are zero than the fourth one is too, so no such term exists.

At next order we look for a term where two of the $\mathbf{k}$'s are zero and two are nonzero. Necessarily the momenta on the remaining two $\mathbf{k}$'s must appropriately sum to zero. We can choose the two non-zero $\mathbf{k}$'s to be both creation, both annihilation, or one of each (which can be chosen in four different ways). Thus the sum of all these terms can be written as

$$\frac{UN_0}{2V}\sum_{\mathbf{k}\neq 0}\left[4\,a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}+a_{-\mathbf{k}}a_{\mathbf{k}}\right] \tag{4.25}$$

We can then look for terms where only one of the $\mathbf{k}$'s is zero. There are such terms, but these will be smaller by a factor of $1/\sqrt{N_0}$ so we throw these out. (In principle at the end of the calculation these terms can be considered as a small perturbation on top of what find).

We then assemble the terms we find. First, the kinetic term from the Hamiltonian Eq. 4.23, secondly, the zeroth order term Eq. 4.24 and the second order term Eq. 4.25. Finally we use one additional trick, we write

$$N_0 = a^\dagger_0 a_0 = N - \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}$$

plugged into the N_0 in Eq. 4.24, we obtain the resulting Hamiltonian

$$H = \frac{U\rho}{2}N + \sum_{\mathbf{k}\neq 0}\left\{\left[\frac{\hbar^2\mathbf{k}^2}{2m}+U\rho\right]a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{U\rho}{2}\left(a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}+a_{-\mathbf{k}}a_{\mathbf{k}}\right)\right\}$$

where $\rho = N/V$. This Hamiltonian is quadratic (and therefore solvable), but it has so-called *anomolous* terms —those with two creation or two annihilation operators. These terms allow particles to scatter in or out of the condensate (the state with $\mathbf{k} = \mathbf{0}$). The scattering terms must conserve total momentum so you can only scatter two-in or two-out at a time.

4.5.1 Bogoliubov Transform

To solve the quadratic hamiltonian with anomolous terms, we invoke the so-called Bogoliubov transformation (invented 1947, by Bogoliubov). Let us write the following transformation

$$\begin{pmatrix} b_{\mathbf{k}} \\ b^\dagger_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \cosh\theta_{\mathbf{k}} & \sinh\theta_{\mathbf{k}} \\ \sinh\theta_{\mathbf{k}} & \cosh\theta_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} a_{\mathbf{k}} \\ a^\dagger_{-\mathbf{k}} \end{pmatrix} \tag{4.26}$$

It is easy to check that if the a's satistfy canonical commutations as in Eqs. 4.3 and 4.4, then the b's similarly satisfy canonical commutations[10]

$$[b_{\mathbf{q}}, b^\dagger_{\mathbf{p}}] = \delta_{\mathbf{q},\mathbf{p}}$$
$$[b_{\mathbf{q}}, b_{\mathbf{p}}] = [b^\dagger_{\mathbf{q}}, b^\dagger_{\mathbf{p}}] = 0$$

---

[10] (Sid's favorite comment): It may look very strange that the matrix in Eq. 4.26 is not a unitary matrix. We know we are allowed to make unitary changes of basis in quantum physics, but non-unitary transforms seem problematic. The reason that this is OK here is because we are making a change of basis on *operators*. If we work out what happens to the resulting *basis states* in the Fock space under this transformation, we will discover that this actually corresponds to a unitary transformation on the Fock space! The only thing we need for this to be true is that canonical commutations are preserved.

Making this transformation (with a bit of algebra **ADD ALGEBRA AS FOOTNOTE OR APPENDIX?**) the Hamiltonian becomes

$$\begin{aligned} H &= \text{const} + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left[\left(\frac{\hbar^2\mathbf{k}^2}{2m}+U\rho\right)\cosh(2\theta_{\mathbf{k}}) - U\rho\sinh(2\theta_{\mathbf{k}})\right]\left[b^\dagger_{\mathbf{k}}b_{\mathbf{k}} + b^\dagger_{-\mathbf{k}}b_{-\mathbf{k}}\right] \\ & \qquad - \left[\left(\frac{\hbar^2\mathbf{k}^2}{2m}+U\rho\right)\sinh(2\theta_{\mathbf{k}}) - U\rho\cosh(2\theta_{\mathbf{k}})\right]\left[b^\dagger_{\mathbf{k}}b^\dagger_{-\mathbf{k}} + b_{-\mathbf{k}}b_{\mathbf{k}}\right] \end{aligned}$$

If we then choose

$$\tanh(2\theta_{\mathbf{k}}) = \frac{U\rho}{\frac{\hbar^2\mathbf{k}^2}{2m}+U\rho} \tag{4.27}$$

we eliminate the anomolous terms and we diagonalize the Hamiltonian, obtaining

$$H = \text{const} + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}}\, b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \tag{4.28}$$

where

$$\begin{aligned} E_{\mathbf{k}} &= +\sqrt{\left(\frac{\hbar^2\mathbf{k}^2}{2m}+U\rho\right)^2 - (U\rho)^2} \\ &\sim \sqrt{\frac{U\rho}{m}}\hbar|\mathbf{k}| + \ldots \qquad \text{for small } \mathbf{k} \end{aligned}$$

Note that this spectrum of excitations in *linear* in **k** at low **k** and then curves to be quadratic at large **k**. Because the dispersion is linear it satisfies the Landau criterion for superfluidity!

The excitations created by the $b^\dagger_{\mathbf{k}}$ operators are sometimes known as *bogoliubons.* The ground state is obviously given by the state with no bogololiubons present

$$b_{\mathbf{k}}|\text{ground state}\rangle = 0 \qquad \text{for all } \mathbf{k}\neq 0$$

Note however, that since we can invert Eq. 4.26, we can write this condition as

$$(\cosh\theta_{\mathbf{k}} a_{\mathbf{k}} + \sinh\theta_{\mathbf{k}} a^\dagger_{-\mathbf{k}})|\text{ground state}\rangle = 0$$

and thus,

$$a_{\mathbf{k}}|\text{ground state}\rangle \neq 0$$

meaning that in the ground state there is some occupation of bosons in $\mathbf{k}\neq 0$ orbitals. As we predicted previously, the interaction has pushed some of the bosons out of the $\mathbf{k}=0$ orbital.

Occupancy of $\mathbf{k} = 0$: Depletion of Condensate

Let us try to calculate how many bosons are in the $\mathbf{k} = 0$ orbital. To do this we write as above

$$N_0 = N - \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$$

so that in the ground state we have

$$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_{\mathbf{k}\neq 0}\langle GS|a^\dagger_{\mathbf{k}} a_{\mathbf{k}}|GS\rangle = 1 - \frac{1}{N}\sum_{\mathbf{k}\neq 0}\sinh^2\theta_{\mathbf{k}} \tag{4.29}$$

with a bit of nasty algebra (detailed in the appendix below) it can be shown that

$$1 - \frac{N_0}{N} \sim U^{3/2}$$

Thus, as we claimed above, for weak interaction, only a few of the bosons are kicked out of the condensate. If U becomes large, then many bosons are kicked out of the condensate and we cannot use this expansion technique.

ODLRO

It is useful to explicitly calculate the off-diagonal-long-ranged-order (ODLRO). First, we write the density matrix (see Eq. 4.19

$$\begin{aligned}\rho_1(\mathbf{r},\mathbf{r}') &= \frac{1}{V}\sum_{\mathbf{k}}\langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \\ &= \frac{N_0}{V} + \frac{1}{V}\sum_{\mathbf{k}\neq 0}\langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \end{aligned} \tag{4.30}$$

Note that if we take $\mathbf{r} = \mathbf{r}'$ the second term is precisely the expression we evaluated for the depletion of the condensate, so that $\rho_1(\mathbf{r},\mathbf{r}) = N/V$ as expected. Here the second term is the Fourier transform of a smooth function which goes to zero for $\mathbf{r}$ far from $\mathbf{r}'$. Thus $\rho_1(\mathbf{r},\mathbf{r}')$ for $\mathbf{r}$ far from $\mathbf{r}'$ goes to N_0/V.

Appendix: Some nasty algebra

To show the previous result, we first note that from Eq. 4.27 we know $\tanh 2\theta$. We then have

$$\text{sech}^2 2\theta = 1 - \tanh^2 2\theta$$

so

$$\frac{1}{\sqrt{1-\tanh^2 2\theta}} = \cosh 2\theta$$

Then we use

$$\frac{1}{2}(\cosh 2\theta - 1) = \sinh\theta$$

so that we obtain

$$\frac{N_0}{N} = 1 - \frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{1-\tanh^2 2\theta_{\mathbf{k}}} - 1\right] = \frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right]$$

Changing the sum to an integral

$$1-\frac{N_0}{N} = \frac{V}{2N}\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right] = 1-\frac{4\pi V}{2N(2\pi)^3}\int_0 k^2 dk\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right]$$

where in the last step we have switched to spherical coordinates. Finally, we rescale variables by defining $k = \sqrt{2mU\rho/\hbar^2}z$ such that we have

$$1 - \frac{N_0}{N} = (\sqrt{2mU\rho/\hbar^2})^3\frac{4\pi V}{2N(2\pi)^3}\int_0 z^2 dz\left[\frac{1}{1-\left(\frac{1}{1+z^2}\right)^2} - 1\right] \sim U^{3/2}$$

as claimed.

Chapter 5

Feynman Theory of Helium-4

For a strongly interacting Bose gas, the Bogoliubov theory fails to be quantitatively accurate, and we need another approach. Feynman came up with a truly ingenious approach[1] for understanding strongly interacting Bose system, with the particular application of superfluid Helium-4 in mind. We will follow this method[2] in order to elucidate the physics of superfluidity further. The question we would like to answer is "what do the low energy excitations of a strongly interacting Bose gas look like?".

5.1 Ground State and Low Energy Excitations

First let us consider the ($T = 0$) ground state for the superfluid at rest in first quantized wavefunction form. we can write it as

$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

This is some very complicated function of the arguments $\mathbf{r}_1, \ldots, \mathbf{r}_N$ since, due to interactions between the bosons, there will be significant correlations between the positions of the particles. Note however, that the wavefunction must be symmetric in exchange of any two particle coordinates by bosonic symmetry.

---

[1] Most people agree that Feynman could easily have been given a Nobel prize for his work on superfluidity, had he not won the prize for quantum electrodynamics.

[2] The Nobel Laureate Murray Gell-Mann joked that Feynman's method consisted of three steps:

1. Write down the problem
2. Think very hard
3. Write down the solution

While obviously he was joking, this does characterize much of Feynman's work. Feynman (similar to Landau) used physical arguments to simply state what the answer has to be, rather than having to perform lengthy calculations (although apparently in private, Feynmann did plenty of lengthy calculations that he then hid from the world to maintain the appearance of being a competely intuitive genius). The negative point of this type of approach is that while it is easy to teach a calculational method, it is hard to teach someone to come up with brilliant physical insights.

Figure 5.1: Compression Waves = Longitudinal Phonon

Even if we don't know the form of the function Φ_0 we can still construct from it a wavefunction for a superfluid flowing. This will take the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \prod_{i=1}^{N} e^{i\theta(\mathbf{r}_i)} \tag{5.1}$$

where $\theta(\mathbf{r})$ is a function of position which must be well defined modulo 2π (and it must be single valued if the amplitude of Φ_0 nowhere vanishes).

For a uniformly flowing supefluid we can choose

$$\theta(\mathbf{r}) = \mathbf{k} \cdot \mathbf{r}$$

for some momentum $\hbar\mathbf{k}$ per particle.

We can check that the velocity of the fluid matches our expectation by looking at the current expectation

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2}\left(\Psi^*\hat{\mathbf{p}}\Psi - (\hat{\mathbf{p}}\Psi^*)\Psi\right)$$

Being that Φ_0 is defined to be the fluid at rest, we must have

$$\mathbf{j}(\mathbf{r})_{\Phi_0} = 0$$

and thus one easily shows that

$$\mathbf{j}(\mathbf{r})_{\Psi} = \hbar n \nabla\theta = n\hbar\mathbf{k}$$

with n the total density, as expected.

Thus given a ground state wavefunction representing a stationary fluid we can write a wavefunction for a flowing superfluid. However, this is not the type of excitation we are interetsted in. So let us now consider low energy excitations given that there is no superflow.

Claim: *In absence of superflow, the only low energy excitations of an interacting Bose gas are (longitudinal) phonons. i.e., compression waves.*

A depiction of compression waves is given in Fig.5.1

We will next argue why this claim is true. We constrast this situation with that of a system of fermions. For fermions (which we will discuss later) the ground state is a Fermi

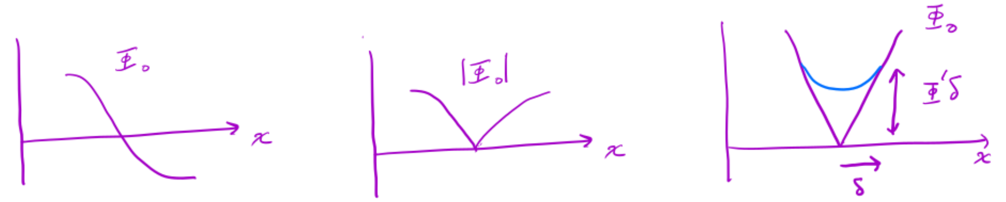

Figure 5.2: Left: A wavefunction Φ_0 which changes sign as a function of some coordinate written as x (but is meant to be some combinations of the positions $\{\mathbf{r}_i\}$. Middle: The absolute value of Φ_0. Except for (the set of measure zero) precisely at the cusp, this gives the same argument in Eq. 5.2 as Φ_0 itself. Right: Smoothing the wavefunction over a scale δ will always reduce the energy a little bit.

sea ($\mathbf{k}$ states filled up to some Fermi surface). In this case we can have many different low energy excitation associated with exciting some fermion from slightly below the Fermi surface to slightly above.

Point 1.1:. *The ground state wavefunction with no superflow, $\Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$, can be chosen real and positive everywhere.*

Firstly, since the Hamiltonian is time-reversal invariant ($H = H^*$), given that the ground state is unique, we must be able to take $\Phi_0 = \Phi_0^*$. Thus we have Φ_0 real. We would now like to show that Φ_0 does not change sign.

Since Φ_0 is assumed to be the ground state, it must minimize the energy

$$\begin{aligned} E &= \langle \Phi_0 | H | \Phi_0 \rangle \qquad (5.2) \\ &= \int \mathbf{dr}_1 \ldots \mathbf{dr}_N \left[\frac{\hbar^2}{2m} \sum_i |\nabla_i \Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i - \mathbf{r}_j) |\Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \right] \end{aligned}$$

We now want to show that Φ_0 for the ground state can always be taken everywhere positive. To show this we first note that if Φ_0 changes sign, then

$$E(\Phi_0) = E(|\Phi_0|)$$

The reason for this is that, as shown in Fig. 5.2, except for positions $\{\mathbf{r}_i\}$ that are a set of measure zero, both $|\Phi_0|^2$ and $|\nabla \Phi_0|^2$ are unchanged if you replace Φ_0 with $|\Phi_0|$. Thus the energy of Eq. 5.2 is unchanged.

Given that Φ_0 and $|\Phi_0|$ have the same energy, let us only consider $|\Phi_0|$ for the moment. Here, we can have a cusp where the wavefunction reaches zero. However, now we argue that we can always reduce the energy of the wavefunction by smoothing the cusp a little bit. Consider smoothing the cusp over a distance scale δ as shown in the right of Fig. 5.2. Let us estimate the energy change from doing this smoothing.

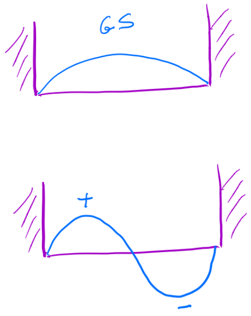

Figure 5.3: Particle in a box. Top: Ground state wavefunction is everywhere positive. Bottom: First excited state — the most positive point is far from the most negative point to minimize the gradient energy.

Roughly, the slope is reduced from $d\Phi_0/dx$ to (say for simplicity) zero, so the kinetic part of the energy (in 1d) (integrating over x) is changed decreased by roughly $\delta(d\Phi_0/dx)^2$. On the other hand, the magnitude of Φ_0 is increased from small (call it zero) to $\delta(d\Phi_0/dx)$. Thus the potential part of the energy is increased proportional to $\delta^3(d\Phi_0/dx)^2$. For small energy δ the decrease in kinetic energy always wins, and we conclude that the ground state Φ_0 can be taken everywhere strictly positive.

Point 1.2: *Any excited state must change sign so that it is orthogonal to the ground state. For a low energy excited state, one must keep gradients small, so the most positive configuration must be "far" from the most negative configuration.*

As a demonstration of this, let us consider the simple quantum mechanical problem of a single particle in a box as shown in Fig. 5.3. The ground state is everywhere postive. The first excited state must change signs to be orthogonal to the ground state. But to keep the gradient energy low, the most positive point (marked + in the figure) must be far from the most negative point (marked - in the figure).

What do these principles mean for a many-particle wavefunction? First, we realize that the first exctited wavefunction must change signs. But again we want to keep gradients small, so that the postive region should be "far" from the negative region. What do we mean by "far" in the case of a many-particle wavefunction? This means "far" in the Nd dimensional parameter space $\{\mathbf{r}_i\}$ (with N the number of particles and d the spatial dimension). We might naively think that we should move all of the particles as far as possible. However, this isn't really correct, because the particles are indistinguishable. Suppose for example, we move all the particles to very far positions as in the left of Fig. 5.4. While this moves every particle "far" from its original position, it is equivalent to a different motion where each particle only moves a small distance, as shown on the right of Fig. 5.4 (due to the fact that the particles are indistinguishable). In fact any motion which leaves the local density unchanged cannot have moved all the particles very far from their original positions.

Figure 5.4: Left: Moving particles "far" from their initial positions. Right: Since particles are indistinguishable, one can get to the same configuration by moving each particle only a little bit.

However, if we were to move all the particles so as to change the density locally, as in Fig. 5.1, this cannot be done simply by moving each particle a small distance – many particles need to be moved a large distance in a way that cannot be reduced by indistinguishibility. Thus two configurations with different density profiles are genuinely "far" from each other in the Nd dimensional parameter space. (Of course changing the density profile *too* much from uniform will be energetically expensive, and cannot be part of a low energy excitation). So we should expect that two different density should correspond to the pieces of the wavefunctions with the most positive and most negative values. (I.e., perhaps the wavefunction takes its most positive value when the configuration looks exactly like Fig. 5.1, and then takes its most negative value when the high and low density regions are interchanged).

Point 2: *A good ansatz for making a low energy excited state from a ground state is to change a single quantum number (to make sure it is orthogonal to the ground state) and try to leave everything else unchanged.*

Suppose we know a ground state Φ_0. We would like to find the lowest energy excited state Ψ which minimizes

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

subject to the constraint of being orthogonal to the ground state

$$\langle \Psi | \Phi_0 \rangle = 0 \tag{5.3}$$

Let us try the approach of the approach proposed in Point 2 on the simple case of the harmonic oscillator.

For a harmonic oscillator we know the ground state is $\Phi_0 \sim e^{-ax^2}$, and the ground state is even parity (reflects around $x = 0$). The simplest way we can change the parity quantum number is just by multiplying the wavefunction by the function x, giving a trial wavefunction $\Psi \sim x\Phi_0$. which has odd parity and then necessarily must satisfy the orthogonality condition Eq. 5.3 on account of having different parity from the ground state. This trial wavefunction is indeed very low energy because qualitatively it is as much like the ground state as it can possibly be, and yet is orthogonal to the ground state (Indeed, in this particular case we have actually guessed the exact first excited state wavefunction!).

Trial Excited State

We thus use the same general idea to write a trial wavefunction for the lowest energy excited state in an interacting Bose gas. We propose the following

$$|\Psi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \rho_{\mathbf{k}} |\Phi_0\rangle \tag{5.4}$$

where Φ_0 is the ground state and $\rho_{\mathbf{k}}$ is the density operator at wavevector $\mathbf{k}$ given explicitly by

$$\begin{aligned} \rho_{\mathbf{k}} &= \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho^\dagger_{-\mathbf{k}} \\ &= \text{Fourier Transform}[\rho(\mathbf{r})] \end{aligned}$$

where

$$\rho(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$$

is the usual density operator.

Let us now list the reasons why this trial excited state wavefunction $|\Psi_{\mathbf{k}}\rangle$ is likely to be an accurate one

1. ρ is symmetric in exchanging particle (switch positions of particles i and j) so $\Psi_{\mathbf{k}}$ has the correct bosonic symmetry.
2. $\rho_{\mathbf{k}}$ changes the momentum quantum number. As described in Point 2 above, this means that the proposed excited state is necessarily orthogonal to the ground state for any $\mathbf{k} \neq \mathbf{0}$.
3. For small $\mathbf{k}$, the operator $\rho_{\mathbf{k}}$ is fairly smooth. This means that multiplying by $\rho_{\mathbf{k}}$ does not ruin any good correlations that are built into the ground state wavefunction Φ_0.
4. The operator $\rho_{\mathbf{k}}$ creates a density wave as in our disucssion in Point 1.2. Taking a simple case where $\mathbf{k}$ is in the $\hat{x}$ direction, we can check that the prefactor $\sum_j e^{ikx_j}$ is maximally positive when all x are of the form $(2\pi/k)n$ for some integer n and it is maximally negative when all x are of the form $(2\pi/k)(n + 1/2)$, corresponding to the two opposite density waves. Of course putting all particles on these particular positions would result in too high a denisty to be low energy, but nonetheless, this argument shows where the wavefunction is positive and where it is negative, and why the positive and negative regions are “far” from each other.
5. The trial wavefunction does not correspond to a superflow (see Eq. 5.1).

6. The trial wavefunction does not change the local density much, so that it should not change the interaction energy much either.
7. Finally (to be shown below) this trial wavefunction matches up with the low energy excitations in Bogoliubov theory which is correct at least in the weak interaction limit.

Let us now confirm item 7, that we would get the same excited state wavefunction in Bogoliubov theory.

First, let us translate the density operator into second quantized notation. We can write

$$\rho(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$$

then Fourier transform using the usual

$$\hat{\psi}^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} a^\dagger_{\mathbf{q}}$$

which allows us to write the Fourier transformed density operator

$$\begin{aligned} \rho_{\mathbf{k}} &= \int \mathbf{dr}\; e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{V} \sum_{\mathbf{q},\mathbf{q}'} e^{-i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{r}} a^\dagger_{\mathbf{q}'} a_{\mathbf{q}} \\ &= \sum_{\mathbf{q}} a^\dagger_{k+q} a_q \end{aligned}$$

Using the same principles we used in section 4.5 the largest terms are those that include the $\mathbf{q} = \mathbf{0}$ modes which are macroscopically occupied. With the usual replacement $a_0, a_0^\dagger \to \sqrt{N_0}$ we obtain

$$\rho_{\mathbf{k}} \sim \sqrt{N_0}\left(a^\dagger_{\mathbf{k}} + a_{-\mathbf{k}}\right)$$

Now from Eq. 4.28 we have that the effective hamiltonian can be written as

$$H = \text{const} + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}}$$

so we can write the low energy excited states as

$$|\Psi_{\mathbf{k}}\rangle = b^\dagger_{\mathbf{k}} |\Phi_0\rangle$$

where Φ_0 is the ground state, meaning the Bogoliubon vacuum. We can, however, also use Eq. 4.26 to rewrite $b^\dagger$ in terms of $a^\dagger$ and a. For small $\mathbf{q}$ we have θ_q in Eq 4.26 being large which means $\sinh\theta \approx \cosh\theta$ and we have

$$b^\dagger_{\mathbf{k}} \sim a^\dagger_{\mathbf{k}} + a_{-\mathbf{k}}$$

Thus for the weakly interacting system, a single bogoliubon excitation is precisely the same as $\Psi_{\mathbf{k}}$ where we just apply the density operator to the ground state!

5.2 Single Mode Excitation Spectrum

So we have proposed a trial wavefunction Eq. 5.4 for the low energy excitations of our interacting Bose gas in terms of the ground state Φ_0. Unfortunately, we do not actually know the ground state Φ_0. Remarkably we can still make progress in calculating the energy of the excited state $\Psi_{\mathbf{k}}$. What we would like to calculate is the energy of the excitation compared to the ground state which we write as

$$\Delta_{\mathbf{k}} = E_{\mathbf{k}} - E_0 = \frac{\langle \Psi_{\mathbf{k}} | H - E_0 | \Psi_{\mathbf{k}} \rangle}{\langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle} \equiv \frac{f(k)}{S(k)} \tag{5.5}$$

where here we have defined the numerator to be called f and the denominator to be called S. Further, we have realized that these quantities will be a function only of the magnitude $k = |\mathbf{k}|$.

Let us attack the denominator first. We have

$$S(\mathbf{k}) = \langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle = \frac{1}{N} \langle \Phi_0 | \rho^\dagger_{\mathbf{k}} \rho_{\mathbf{k}} | \Phi_0 \rangle$$

this quantity is known as the *structure factor*, and it is directly measured by x-ray and neutron scattering[3]. We can simplify this result by using

$$\rho_{\mathbf{k}} = \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho^\dagger_{-\mathbf{k}} \tag{5.6}$$

We then obtain[4]

$$\begin{aligned} S(\mathbf{k}) = \langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle &= \frac{1}{N} \left\langle \Phi_0 \left| \textstyle\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \right| \Phi_0 \right\rangle \\ &= \frac{1}{N} \left\langle \Phi_0 \left| \textstyle\sum_{i,j} e^{-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right| \Phi_0 \right\rangle \\ &= \text{Fourier Transform} \left[\left\langle \Phi_0 \left| \textstyle\sum_{i,j} \delta(\mathbf{r} - (\mathbf{r_i} - \mathbf{r_j})) \right| \Phi_0 \right\rangle \right] \end{aligned}$$

Experimental neutron diffraction measurements of the structure factor of Helium-4 are given in Fig. 5.5 The peak in the structure factor is roughly the analog of a Bragg peak for a crystal — it occurs at a wavevector of roughly $2\pi/a$ where a is the typical inter-particle spacing.

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[3] This is not quite the same structure factor we study in our elementary solid state courses when we study scattering from crystals, although it is very closely related. See next footnote

[4] In elementary solid state physics courses, we define the structure factor to be

$$\tilde{S}(\mathbf{k}) \sim \langle \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \rangle,$$

and the scattering intensity is $\sim |\tilde{S}|^2$. However, in a fluid this $\tilde{S}(\mathbf{k})$ is zero for any $\mathbf{k} \neq 0$ since all positions are equally likely. Instead we are now calulating the expectation of the square of this quantity, with the average outside of the square.

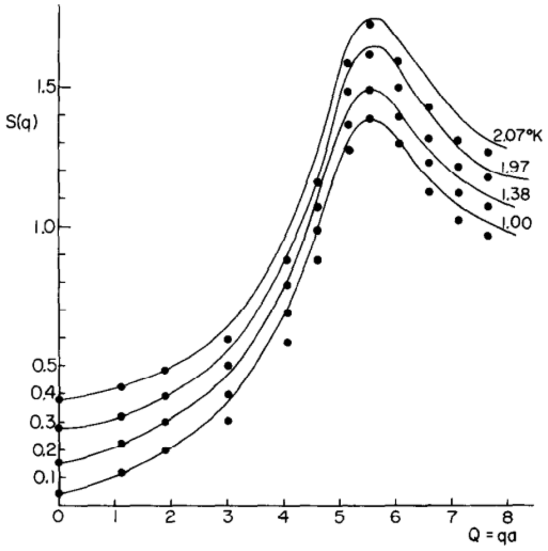

Fig. 1. Structure factor of liquid helium at various temperatures. The dots represent what Sears, Svensson, Woods and Martel have given [9].

Figure 5.5: The structure factor of superfluid Helium. Figure from A. Isihara, Physica 106B (1981) 161-164.

Let us now turn to the numerator of Eq. 5.5. We have

$$\begin{aligned} f(\mathbf{k}) &= \frac{1}{N}\left\langle \Phi_0|\rho^\dagger_{\mathbf{k}}(H-E_0)\rho_{\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{1}{N}\left[\left\langle \Phi_0|\rho^\dagger_{\mathbf{k}}H\rho_{\mathbf{k}}|\Phi_0\right\rangle - \left\langle \Phi_0|\rho^\dagger_{\mathbf{k}}\rho_{\mathbf{k}}H|\Phi_0\right\rangle\right] \\ &= \frac{1}{N}\left\langle \Phi_0|\,\rho^\dagger_{\mathbf{k}}\,[H,\rho_{\mathbf{k}}]|\Phi_0\right\rangle \end{aligned} \tag{5.7}$$

where in going to the second line used the fact that the Φ_0 is an eigenvalue with eigenenergy E_0.

On the other hand, we equivalently could have written

$$\begin{aligned} f(\mathbf{k}) &= \frac{1}{N}\left\langle \Phi_0|\rho^\dagger_{\mathbf{k}}(H-E_0)\rho_{\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{1}{N}\left[\left\langle \Phi_0|\rho^\dagger_{\mathbf{k}}H\rho_{\mathbf{k}}|\Phi_0\right\rangle - \left\langle \Phi_0|H\rho^\dagger_{\mathbf{k}}\rho_{\mathbf{k}}|\Phi_0\right\rangle\right] \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho^\dagger_{\mathbf{k}}]\,\rho_{\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho^\dagger_{-\mathbf{k}}]\,\rho_{-\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho_{\mathbf{k}}]\,\rho^\dagger_{\mathbf{k}}|\Phi_0\right\rangle \end{aligned} \tag{5.8}$$

where in going to second last line we have used the fact that, due to isotropy of the fluid we expect $f(\mathbf{k}) = f(-\mathbf{k})$ and in going to the last line we use that $\rho_{\mathbf{k}}^\dagger = \rho_{-\mathbf{k}}$.

Putting together Eq. 5.7 and 5.8 we obtain the double commutator form

$$f(\mathbf{k}) \;=\; \frac{1}{2N}\left\langle \Phi_0 \left| \left[\rho_{\mathbf{k}}^\dagger, [H, \rho_{\mathbf{k}}]\right] \right| \Phi_0 \right\rangle \tag{5.9}$$

We now must determine the double commutator, which will turn out to be a simple number rather than an operator! To do this we notice recall the Hamiltonian has three terms, a kinetic term $\hat{K}$, a one body potential term $\hat{V}$ and a two body interaction term $\hat{U}$ (it would not matter if we had three or four body terms etc). We write

$$H = \hat{K} + \hat{V} + \hat{U}$$

where

$$\begin{aligned}
\hat{K} &= \sum_i \frac{-\hbar^2 \nabla_i^2}{2m} \\
\hat{V} &= \sum_i V(\mathbf{r}_i) \\
\hat{U} &= \frac{1}{2}\sum_{i,j} U(\mathbf{r}_i - \mathbf{r}_j)
\end{aligned}$$

And recall that

$$\rho_{\mathbf{k}} = \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho_{-\mathbf{k}}^\dagger \tag{5.10}$$

We now want to calculate $[H, \rho_k]$. Here ρ only contains the operator $\mathbf{r}$ (not the conjugate operator ∇) and this then commutes with both U and V which also only contain $\mathbf{r}$ (and not ∇). However, ρ_k does not commute with the kinetic term, so we simplify

$$\begin{aligned}
[H, \rho_k] &= [\hat{K}, \rho_k] \\
&= \left[\sum_i \frac{-\hbar^2 \nabla_i^2}{2m} \, , \, \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \right] \\
&= \frac{-\hbar^2}{2m} \sum_j \left[\nabla_j^2 \, , \, e^{i\mathbf{k}\cdot\mathbf{r}_j} \right] \\
&= \frac{-\hbar^2}{2m} \sum_j \left(-\mathbf{k}^2 + 2i\mathbf{k}\cdot\nabla_j \right)
\end{aligned}$$

We then want to further calculate the double commutator

$$\left[\rho_{\mathbf{k}}^\dagger \, , [H, \rho_{\mathbf{k}}]\right] \;=\; \frac{-\hbar^2}{2m} \sum_j \left[\rho_{\mathbf{k}}^\dagger \, , \left(-\mathbf{k}^2 + 2i\mathbf{k}\cdot\nabla_j \right) \right]$$

The $-\mathbf{k}^2$ term is a scalar so it commutes and we have

$$\begin{aligned}
\left[\rho_{\mathbf{k}}^{\dagger}, [H, \rho_{\mathbf{k}}]\right] &= \frac{-\hbar^2}{m}\sum_j \left[\rho_{\mathbf{k}}^{\dagger}, (i\mathbf{k}\cdot\nabla_j)\right] \\
&= \frac{-\hbar^2}{m}\sum_j \left[\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}, (i\mathbf{k}\cdot\nabla_j)\right] \\
&= \frac{-\hbar^2 N}{m}\left[e^{-i\mathbf{k}\cdot\mathbf{r}}, (i\mathbf{k}\cdot\nabla)\right] \\
&= \frac{\hbar^2\mathbf{k}^2 N}{m} \qquad (5.11)
\end{aligned}$$

which is simply a scalar rather than an operator, as claimed. Thus plugging into Eq. 5.9 we obtain

$$f(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m}$$

We note that this double commutator calculation is used in several other common contexts, such as in the derivation of the well-known f-sum rule, and Kohn's theorem. (Don't worry if you don't know about these! We will run into it again in section 8.3.2 below).

Now plugging back into our original formula for the excitation energy, Eq. 5.5 we have

$$\Delta_{\mathbf{k}} = \frac{f(k)}{S(k)} = \frac{\hbar^2 k^2}{2mS(k)} \qquad (5.12)$$

This is a rather remarkable result! In this approxiation[5], the low energy excitation spectrum is completely determined by the structure factor!

In Fig. 5.6 the top curve is the prediction of the Feynman theory using Eq. 5.12 with the experimentally measured structure factor $S(k)$ as input. The bottom curve is the experimentally measured excitation spectrum (using inelastic neutron scattering). The structure of the two curves is quite similar.

Note that in the long wavelength (small k) limit the Feynman theory matches the experimental results exactly. At higher k, the Feynman theory gives an excitation energy which is higher than the real excitation energy. This is to be expected. In fact, the Feynman theory can be taken to be a rigorous upper bound: What we have done is a variational calculation using $\rho_k|\Phi_0\rangle$ as the trial state — even though this isn't exactly the eigenstate (except in the long wavelength limit where it becomes exact). In the space of states orthogonal to the ground state, the exact state we are looking for is the lowest energy state, so our trial state is necessarily higher in energy than the exact state.

The minimum in energy at intermediate k is known as the *roton* minimum, and it corresponds (approximately) to the peak in the structure factor (See Fig. 5.5) at k roughly $2\pi/a$ with a the interparticle spacing.

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[5] It is an approximation here because we are using a trial wavefunction for the excited state.

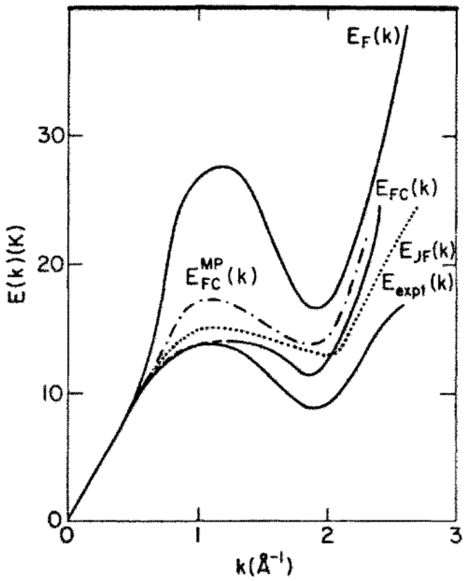

FIGURE 3.7. *Comparison of Jackson and Feenberg (1962) variational calculation of the excitation spectrum of liquid He II with prior calculations and with experiment.*

Figure 5.6: Feynman Theory and Low energy excitations of Helium. Figure from Pines and Nozieres. Top curve is prediction of Feynman theory. Bottom curve is experimental measurement of the excitation spectrum. Curves in between are modifications of the Feynman theory.

In fact, Landau predicted this minimum before Feynman's theory. He based his prediction on specific heat data. Knowing that the spectrum is linear $E(k) = \hbar vk$ at small k, the usual Debye calculation gives a specific heat $C_v \sim T^3$ at low T. However, the experiments showed at higher T an additional contribution that appeared to turn on roughly as $\sim e^{-E_r/(k_b T)}$ for some constant E_r. Landau relized that a spectrum of the shape shown in Fig. 5.6 would give such a term where E_r is the energy of the roton minimum.

Chapter 6

Ginzburg-Landau Theory

6.1 Neutral Superfluids

Let us begin by recalling the Gross-Pitaevskii energy we derived earlier for weakly interacting (uncharged) Bose gases in Eq. 4.13 which we rewrite here

$$\langle H \rangle = \int d\mathbf{r} \left(\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{U}{2}|\psi(\mathbf{r})|^4 \right) \tag{6.1}$$

To anyone who has studied the Landau theory of phase transitions (and the associated Ginzburg-Landau[1] theory of fluctuations) this form is not surprising. Near a phase transition we typically expand a free energy order by order, writing down all terms that are allowed by symmetry. In the case of a neutral superfluid with a complex order parameter we generally expect a free energy functional of the form

$$F[\psi(\mathbf{r})] = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} |\nabla \psi|^2 + \alpha_2 |\psi|^2 + \alpha_4 |\psi|^4 \right] \tag{6.2}$$

where $|\psi|^2$ is interpreted as the superfluid density[2]. Not only does this agree with Gross-Pitaevskii, but on symmetry grounds, this must be the form of the free energy near the phase transition.

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[1] Vitali Ginzburg won a Nobel prize in 2003 for his eary work in the 1950s on what is now called the Ginzburg-Landau theory of superconductors. (We will come to this later in the current chapter). Ginzburg's Nobel biography is well worth a read — as a Jew in Stalin's USSR, he barely skirted death on several occassions!

[2] Generally we might have thought that the coefficient of the gradient term might have been an arbitrary fit parameter, but we fix it using the fact that if we write $\psi = |\psi| e^{i\mathbf{k}\cdot\mathbf{x}}$ we want $\hbar\mathbf{k}$ to represent a particle momentum.

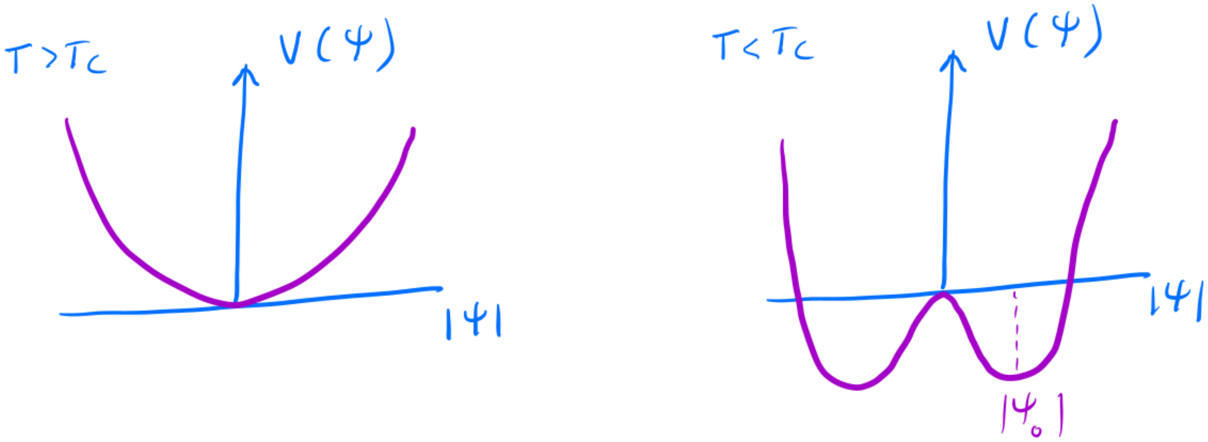

Figure 6.1: Left: The Ginzburg-Landau potential above T_c. Here the minimum is at $\psi = 0$ indicating no superfluid density. Right: The Ginzburg-Landau potential below T_c. Here the minimum is at a nonzero value of ψ indicating finite superfluid density.

6.1.1 Spatially Uniform Solution

To begin with, let us consider a uniform system — so that the gradient is zero. As in the usual theory of phase transitions we have

$$\alpha_2 = a(T - T_c)$$

with $a > 0$ and $\alpha_4 > 0$ as well for stability (i.e, so that for large enough ψ the free energy always increases.

Often we will think of the non-gradient terms of the free energy as being a potential

$$\begin{aligned} V(\psi) &= \alpha_2|\psi|^2 + \alpha_4|\psi^4| \\ &= a(T - T_c)|\psi|^2 + \alpha_4|\psi^4| \end{aligned}$$

with $a > 0$.

For $T > T_c$ (so $\alpha_2 > 0$) the potential $V(\psi)$ looks like the left of Fig. 6.1, where the minimum is at $|\psi| = 0$ meaning that the ground state has no supefluid density.

On the other hand, for $T < T_c$ (so $\alpha_2 < 0$) the minimum is at some finite nonzero value of $|\psi|$ (which we label ψ_0) meaning there is a finite superfluid density ψ_0^2 in the ground state.

It is simple to minimize $V(|\psi|)$ to obtain

$$|\psi|^2 = \frac{|\alpha_2|}{2\alpha_4} = \psi_0^2 = n_s \tag{6.3}$$

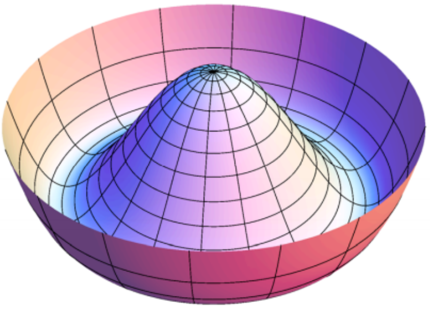

Figure 6.2: Left: The Ginzburg-Landau potential below T_c drawn as a function of the complex (2d) field ψ. The two orthogonal directions in the horizontal plane can be taken to be the real and imaginary parts of ψ. The minimum lies at the bottom of the trough (the bottom of the rim of the hat)

which is the density of the superfluid fraction.

Since ψ is actually a complex field, it should really be drawn as the so-called Mexican hat potential shown in Fig. 6.2. Note that the potential $V(\psi)$ is a function of $|\psi|$ only and is independent of the complex phase of ψ. This means that the ground state is degenerate — the ground state has magnitude ψ_0 but all possible complex phases have the same energy. In Fig. 6.2 we see this as the symmetry of the picture under rotation around the central z-axis. In particular, the minimum of the potential is a (degenerate) circle around the bottom of the rim of the Mexican hat.

Whenever we have multiple global ground states related to each other by a continuous symmetry (the result of spontaneously broken continuous symmetry) we should have a Goldstone boson (or "Nambu-Goldstone" boson[3]). The boson in this case is the low energy excitation associated with the ground state locally reorienting this degree of freedom. In this case the Goldstone boson is nothing more than phase fluctuations of ψ (without changing the magnitude of ψ). In other words, the phase changes slowly as a function of position. These excitations are the superfluid phonons, or bogoliubon excitations.

6.1.2 Spatial Dependence: Ginzburg Landau Theory

Let us now return to the free energy Eq. 6.2 and reintroduce the spatial derivative (i.e., no longer assume ψ has no spatial dependence). Here we will assume we are in the superfluid phase, i.e., $T < T_c$. To derive an equation for ψ we take the functional derivative of Eq. 6.2

---

[3] Named for Yoichiro Nambu, a Nobel Laureate, for his work on spontaneous symmetry breaking, and Jeffrey Goldstone, who generalized Nambu's discovery. Nambu joked that he won the Nobel prize mainly by outliving his enemies. He was 87 when he won the prize.

to minimize the free energy

$$\begin{aligned}\frac{\delta F}{\delta \psi^*} &= 0 \\ -\frac{\hbar^2}{2m}\nabla^2\psi + \alpha_2\psi + 2\alpha_4|\psi|^2\psi &= 0\end{aligned}$$

which is a non-linear Schroedinger equation (See Eq. 4.13). Recalling that in a uniform system below T_c we have $|\psi_0|^2 = |\alpha_2|/(2\alpha_4)$, it is useful to define a new field

$$f = \psi/|\psi_0|$$

so that in the uniform system we just have $f = 1$.

Writing $\psi = f|\psi_0|$ and plugging into our nonlinear Schroedinger equation we obtain

$$-\frac{\hbar^2}{2m}\nabla^2 f + \alpha_2 f + 2\alpha_4|\psi_0|^2|f|^2 f = 0 \tag{6.4}$$

Dividing through by α_2 and using $|\psi_0|\alpha_4 = |\alpha_2|/2$ we obtain

$$\xi^2\nabla^2 f + f - f|f|^2 = 0 \tag{6.5}$$

where

$$\xi = \sqrt{\frac{\hbar^2}{2m|\alpha_2|}} \tag{6.6}$$

is known as the Ginzburg-Landau coherence length. This is the natural length scale associated with the nonlinear Schroedinger equation. It is effectively a stiffness length for twising the phase or magnitude of the field ψ.

At low temperatures, the Ginzburg-Landau coherence length for superfluid ^{4}He is on the order of $\xi \approx 1$ Angstrom. However, note that at the critical temperature $\alpha_2 = a(T - T_c)$ changes sign (therefore going through zero) so as we approach T_c we must have ξ diverging as

$$\xi \sim |T - T_c|^{-1/2}$$

Note that Ginzburg-Landau theory is a mean field theory. A more accurate analysis of the problem will obtain a different exponent[4].

Despite the fact that our equation is nonlinear (and therefore hard to solve) some exact solutions are in fact possible.

Solution 1. Uniform solution:

$$f = 1 \quad \text{everywhere}$$

---

[4] This is 3d, XY universality class and $\nu = .671...$

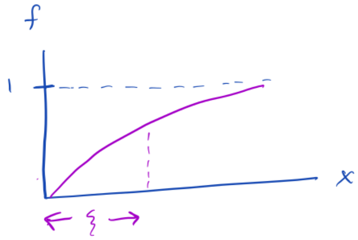

Figure 6.3: The healing of the order parameter from a hard wall is a tanh function.

(This one is obvious)

Solution 2. Hard wall boundary condition: We

$$f = \tanh\left(\frac{x}{\sqrt{2}\xi}\right) \tag{6.7}$$

This solution, shown roughly in Fig.6.3

$$\begin{aligned} f &\to 1 \qquad \text{at large } x \\ f &\to 0 \qquad \text{at } x \to 0 \end{aligned}$$

The proof that the tanh form in Eq. 6.7 satisfies the nonlinear Schroedinger equation 6.5 is a bit of an exercise in hypergeometric functions. We leave this to the reader.

Solution 3. A Single Vortex

We consider a vortex line going along the z-axis. In cylindrical coordinates, we impose

$$f = |f(r)|e^{i\theta}$$

Plugging this into our nonlinear Schroedinger Equation 6.5, using

$$\nabla^2 f = \left[\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial \theta}\right)\right] f$$

we obtain

$$\xi^2 \left[\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} - \frac{1}{r^2}\right] |f| + |f| - |f|^3 = 0$$

This leaves us with something that is unfortunately not analytically solvable. However, we can obtain two limits.

Small r: First, if we consider small r, we know that f needs to vanish as $r \to 0$. Thus we can throw out $|f|^3$ term. We then focus on the most singular terms which are those within the brackets. It is clear these can be made zero by using

$$|f| = \alpha r + \dots$$

where the ... terms are terms higher order in r which one obtains when you reinstate the terms we just threw out. Thus we conclude that $|f| \sim r$ for small r

Large r: We know far from a vortex, we should get the bulk solution $|f| = 1$ so we look for a perturbation to this by substituting $|f| = 1 - y$. Keeping only terms linear in y and looking in the large r limit where the derivatives are suppresed we obtain

$$y = \xi^2/(2r^2) + \ldots$$

so

$$|f| = 1 - \xi^2/(2r^2) + \ldots$$

6.2 Charged Superfluids (i.e., Superconductors)

The same approach can be applied to charged superfluids with the additional complication that we need to keep to keep track of the electromagnetic field. We can write a free energy functional now in the form

$$\begin{aligned} F[\psi, \mathbf{E}, \mathbf{B}] &= \int d\mathbf{r} \left[\frac{1}{2m^*} |(-i\hbar\nabla - e^*\mathbf{A})\psi|^2 + \alpha_2|\psi|^2 + \alpha_4|\psi|^4 \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.8}$$

and as usual $\alpha_4 > 0$ and $\alpha_2 = a(T - T_c)$ with $a > 0$. Here we have minimally coupled the momentum operator to the vector potential, and we have added the usual energy of an electromagnetic field (the second line). Note that the integral on the second line has a prime on it, this is to point out that integral of the electromagnetic field extends over all of space – the field energy still needs to be considered in regions outside of the physical sample, which may be finite.

As in the case of the neutral superfluid, below T_c we have

$$|\psi| = \psi_0 = \sqrt{\frac{|\alpha_2|}{2\alpha_4}} = \sqrt{n_s^*}$$

with n_s^* the number of particles in the superfluid (superconducting) fraction (where here we are assuming a uniform solution with no applied vector potential to make more precise analogy with the neutral superfluid).

6.2.1 Anderson-Higgs Mechanism

As in the case of the neutral superfluid, one might expect that there would be a Goldstone mode associated with changing the phase of the order parameter — i.e., moving the field around the rim of the Mexican hat as a function of position. But in fact, there is no such low energy mode of the superfluid in a superconductor! This is due to the so-called "Anderson-Higgs" mechanism[5] which we will now discuss.

It is perhaps more natural to discuss the Higgs mechanisms in terms of Lagrangians rather than free energies — since that makes it easier to keep track of dynamics[6]. However, so far we have been working in terms of free energies, and we will therefore continue using this approach since it is easier to compare to what we have done earlier.

First we note that the free energy is invariant under the gauge transform:

$$\begin{aligned} \psi &\rightarrow e^{i\alpha}\psi \\ e^*\mathbf{A} &\rightarrow e^*\mathbf{A} + \nabla\alpha/\hbar \end{aligned}$$

with α real. This gauge transform can be a function of both time and position $\alpha(t, \mathbf{r})$.

Recalling that for $T < T_c$ we have

$$|\psi| = \psi_0 = \sqrt{\frac{|\alpha_2|}{2\alpha_4}}$$

which minimizes the potential $V(\psi)$. Here ψ_0 is the so-called Vacuum Expectation Value of the field, or VEV in high-energy language. Let us now consider fluctuations around this minimum.

We write

$$\psi = (\psi_0 + h)e^{i\chi} \tag{6.9}$$

where h and χ are both real. Here, h is the fluctuation of the magnitude of ψ, and χ is fluctuation of the angle around the "rim" of the Mexican hat. Near the bottom of the rim the energy should be quadratic in h describing deviation up the hill and away from the bottom of the rim. Inedeed,

$$\alpha_2|\psi|^2 + \alpha_4|\psi|^4 = \alpha_2(\psi_0 + h)^2 + \alpha_4(\psi_0 + h)^4 = \text{const} + 2|\alpha_2|h^2 + \ldots$$

Now we would like to plug Eq. 6.9 into the free energy Eq. 6.8. However, before doing this, let us choose a gauge that absorbes the phase χ in Eq. 6.9. I.e., we gauge transform to make ψ real

$$\begin{aligned} \psi &\rightarrow \psi' = e^{-i\chi}\psi = \psi_0 + h \\ e^*\mathbf{A} &\rightarrow e^*\mathbf{A}' = e^*\mathbf{A} - \hbar\nabla\chi \end{aligned} \tag{6.10}$$

---

[5] Perhaps the history of the Higgs mechanism starts with Nambu, who wrote a key paper in 1960 starting to understand the ideas of spontaneous breaking of a gauge symmetry. Then in 1962, Anderson fully described what we now call the Higgs mechanism in the context of superconductors. In 1964, in Higgs' first paper (in the first paragraph) he credits Anderson saying (a) This is nothing more than extending what Anderson did to the electro-weak interactions and (b) Anderson himself suggested that a similar mechanism might exist in high energy. More detailed papers appeared the same year expanding further on the idea by Brout and Englert; and by Guralnik, Hagen, and Kibble. Anderson probably was entitled to part of the Nobel shared by Higgs and Englert (Brout had passed away before the prize was awarded), but Anderson already had a prize for what is now called "Anderson Localization", which is totally unrelated (except for the fact that both require someone very smart to figure them out).

[6] For those who want to write a Lagrangian, we simply consider F to be the Hamiltonian and write a Lagrangian density as $\mathcal{L} = |\partial_t\psi|^2 - \mathcal{H}$ with $\mathcal{H}$ the Hamiltonian density.

With this transformation we have

$$\begin{aligned} F &= \int d\mathbf{r} \left[\frac{1}{2m^*} |(-i\hbar\nabla - e^*\mathbf{A}')(\psi_0 + h)|^2 + 2|\alpha_2| h^2 \, + \ldots \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.11}$$

Note that both the electric and magnetic fields corresponding to $\mathbf{A}'$ are the same as those corresponding to $\mathbf{A}$ (the fields are *gauge invariant*).

This free energy can be rewritten as

$$\begin{aligned} F &= \int d\mathbf{r} \left[\left(\frac{\hbar^2}{2m^*} |\nabla h|^2 + 2|\alpha_2| h^2 \right) + \frac{\psi_0^2 (e^*)^2}{2m^*} \mathbf{A}'^2 \, + \ldots \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.12}$$

One might naively expect there would have been terms $i(\nabla h) \cdot \mathbf{A}'$ but such terms have to cancel on account of being imaginary (they do!).

Let us first consider the terms involving h. This field is *massive*, meaning that there are no low energy excitation, the mass here being given by the α_2 term[7].

The term with $\mathbf{A}'^2$ represents a mass for the electromagnetic photon. Like the h^2 term, this term gives a finite energy to any nonzero value of the electromagentic field, and hence is a mass. We should compare this to the case of conventional electromagnetism where we have only the $\mathbf{B}^2$ and $\mathbf{E}^2$ terms.

$$\begin{aligned} \mathbf{B}^2 &= (\nabla \times \mathbf{A})^2 \\ \mathbf{E}^2 &= (-\nabla A_0 - \partial_t \mathbf{A})^2 \end{aligned}$$

Since both of these have derivatives, the energy of the electromagnetic field goes to zero at long wavelength (we should know this since the energy of a photon is $2\pi\hbar c/\lambda$). However, now with the $\mathbf{A}'$ term added, the energy of a photon is finite even at very long wavelenth.

What does it mean that the photon is massive? What is means is that even a long wavelength photon costs energy when it is inside a superconductor. If we imagine a photon outside a superconductor, when it tries to go into the superconductor it will experience an energetic barrier and will be repelled — this is precisely the Meissner effect: electromagnetism is expelled from superconductors!

What has happened here? The so-called Higgs mechanism is this process by which the Goldstone mode associated with the phase of the order parameter disappears (we got rid of it by absorbing the phase in Eq. 6.10), but in the process the photon becomes massive[8]. Note also that where a massless photon has only two polarizations (due to the

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[7] To see this, we see that any nonzero value of h gives a positive energy. The lowest energy we can get for a normalized function $h(\mathbf{r})$ is $2|\alpha_2|$ if h is uniform in space.

[8] The easy to remember catch phrase is that the gauge boson has become massive because it ate the goldstone boson... with the obvious reference being that one becomes massive when one eats. There may be other mechanisms by which the gauge boson gets some exercise and loses weight (that is a joke).

$T > T_c$		$T < T_c$
Oscillations of ψ in real and complex direciton		Oscillation of h in real direction only
2 polarizations of massless photon		3 polarizations of massive photon
4 total degrees of freedom	=	4 total degrees of freedom

Table 6.1: Conservation of total number of degrees of freedom in the Higgs mechanism.

fact that it moves at the speed of light), a massive photon which moves slower than the speed of light (like a phonon) has three possible polarizations — inlcuding a longitudinal mode. Thus, although we lose a degree of freedom from the oscillation of the field ψ, we gain a degree of freedom in a new oscillation mode of the photon. As shown in Table 6.1 the total number of degrees of freedom is the same above and below T_c.

One comment I feel compelled to add before leaving the discussion of Higgs mechanism: Particularly in the media, one often hears people say that the Higgs boson "gives" mass to particles[9]. This is not true. The Anderson-Higgs boson in this case is the field h. However, it is the vacuum expectation value (VEV) ψ_0 that gives mass to photon. The Higgs boson represents the oscillations of the ψ field that remain once it has aquired a VEV (And further these oscillations become massive since the massless goldstone mode disappeared when we fixed the phase).

6.2.2 Equations of Motion

As in our Gross-Pitaevskii approach, one can differentiate the free energy to obtain equations of motion.

$$\frac{\delta F}{\delta \psi^*} = 0$$

yielding the nonlinear Schroedinger equation coupled to a vector potential

$$\left[\frac{1}{2m^*}(-i\hbar\nabla - e^*\mathbf{A})^2 + \alpha_2 + 2\alpha_4|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = 0$$

Similarly we can differentiate with respect to the vector potential in our fixed gauge

$$\frac{\delta F}{\delta A_\mu} = 0$$

and after some exercize in functional differentiation we obtain

$$\frac{\nabla \times \mathbf{B}}{\mu_0} - \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \frac{e^*}{2m^*}\left[\psi^*\left\{(\mathbf{p} - e^*\mathbf{A})\psi\right\} - \left\{(\mathbf{p} + e^*\mathbf{A})\psi^*\right\}\psi\right]$$

and from Maxwell's equation on the left we can identify that the right hand side must be the electrical current density **j** as we had previously claimed. If the ground state ψ is

---

[9] It is also often said that the Higgs mechanism gives mass to all the particles in the universe. This is also not true. Hadrons get their mass mainly from gluon energy!

uniform, we thus recover the London equation

$$\mathbf{j} = \frac{(e^*)^2}{m^*}|\psi|^2 \mathbf{A} = \frac{(e^*)^2}{m^*} n_s^* \mathbf{A}$$

where we have now identified $|\psi|^2$ to be the superfluid density.

6.2.3 Energetics from Ginzburg-Landau theory: Type I and Type II superconductors revisited

From the Ginzburg-Landau potential

$$V(\psi) = \alpha_2 |\psi|^2 + \alpha_4 |\psi|^4$$

recall from Eq. 6.3 that we derived that the minimum free energy occurs at

$$|\psi|^2 = \psi_0^2 = \frac{|\alpha_2|}{2\alpha_4} = n_s^*$$

where we have identified this quantity as the superfluid density (we have inserted the * as previously to again indicate that we do not know how many electrons might be bound together to form one boson).

Recall also from Eq. 3.8 the London penetration depth is given by

$$\lambda = \sqrt{\frac{m^*}{(e^*)^2 n_s^* \mu_0}} = \sqrt{\frac{2\alpha_4 m^*}{(e^*)^2 |\alpha_2| \mu_0}} \tag{6.13}$$

which gives us the decay length of a magnetic field when it penetrates into a superconductor.

On the other hand, we also derived in Eq. 6.6 a phase stiffness length (or coherence length)

$$\xi = \sqrt{\frac{\hbar^2}{2m^* |\alpha_2|}} \tag{6.14}$$

Note that both of these lengths scale as

$$\xi \text{ and } \lambda \sim \frac{1}{\sqrt{|\alpha_2|}} \sim |T - T_c|^{-1/2} \tag{6.15}$$

when we are close to T_c.

Note that this exponent of $-1/2$ is a so-called *mean-field* exponent. A more careful renormalization group calculation will give a different exponent. However, it turns out

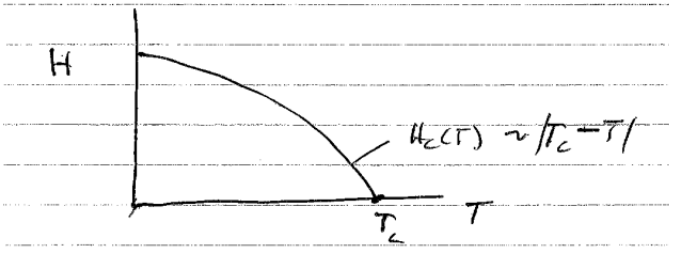

Figure 6.4: The critical field scales linearly with $T - T_c$ close to T_c, at least within a mean field theory calculation.

that mean field theory tends to be extremely good for superconductors, except when one gets exceedingly close to the critical temperature[10].

The free energy density is given by

$$\begin{aligned} \min(F)/V = F[\psi_0]/V &= \alpha_2|\psi_0|^2 + \alpha_4|\psi_0|^4 \\ &= \frac{-\alpha_2^2}{4\alpha_4} \end{aligned} \tag{6.16}$$

This energy is the energy that is gained by allowing ψ_0 to become nonzero — i.e., it is the condensation energy per unit volume. Back in Eq. 3.18 we already calculated the condensation energy per unit volume and using thermodynamics we related it to the critical field H_c as

$$\text{condensation energy per volume} = \frac{\mu_0 H_c^2}{2} = \frac{\alpha_2^2}{4\alpha_4}$$

Thus in terms of the Ginzburg-Landau parameters we obtain

$$H_c = |\alpha_2|\sqrt{\frac{1}{2\mu_0\alpha_4}} \sim (T - T_c) \tag{6.17}$$

as shown in Fig. 6.4

In Eq. 6.17 we have the combination $|\alpha_2|/\sqrt{\alpha_4}$ and it is useful to try to construct this combination out of the known quantities of the coherence length ξ in Eq. 6.14 and the penentration depth λ in Eq. 6.13. If we take the combination

$$\frac{1}{\xi\lambda} = \frac{|\alpha_2|}{\sqrt{\alpha_4}}\left(\frac{e^*}{\hbar}\right)\sqrt{\mu_0} \quad ,$$

---

[10] The reason that mean field theory works so well is that that the coherence length ξ in a superconductor is extremely large compared to micscopic length scales. The typical fluctations are of energy k_bT over a size ξ^D with D the dimensionality of space giving an energy density for the fluctuations of $k_BT/\xi^D \sim |T - T_c|^{D/2}$. We should compare this mean fluctuation energy to the mean field ground state energy density which is $\alpha_2^2/(4\alpha_4) \sim |T - T_c|^2$ (See Eq. 6.16). Close enough to T_c the fluctuation always becomes larger than the mean field energy (for $D < 4$) so mean field theory always fails. However, if the prefactor y in $\xi = y|T - T_c|^{-1/2}$ is extremely large, as it is in superconductors, then one must go very close to T_c before this failure happens.

H_c H_{c1}

Figure 6.5: Pictoral Descriptions of Critical Fields. Left: H_c can be described as a field such that one flux quantum penetrates a box of size λ by ξ. Right: H_{c1} can be described as a field such that one flux quantum penetrates a box of size λ by λ.

we note that a factor of $2m^*$ has cancelled here. Recalling that the superconducting flux quantum is $\phi_0 = 2\pi\hbar/(e^*)$ we can rearrange the prior two equations to get

$$H_c = \frac{1}{\xi\lambda}\,\frac{\phi_0}{2\pi\mu_0\sqrt{2}} \tag{6.18}$$

What this means is that if we draw a box of area λ on one side and ξ on the other side, H_c, the magnetic field necessary to completely destroy superconductivity, is the magnetic field where we have roughly one flux quantum penetrating this area as shown in the left of Fig. 6.5.

Now recall from the end of section 3.1.5 that the distinction between Type I and Type II superconductors depends on the energy per unit length ϵ, or "tension" of a vortex line. To remind you we have the lower critical field (where magnetic field first can penetrate a superconductor)

$$H_{c1} = \frac{\epsilon}{2\phi_0}$$

and if this quantity is lower than H_c then we have a Type II superconductor with a vortex (Abrikosov) phase for $H_{c1} < H < H_{c2}$, but if $H_{c1} > H_c$ then no vortex phase exists. It is thus useful to try to make an estimate of the vortex line tension ϵ, or energy per unit length of the vortex.

Roughly the energy of a vortex is due to the fact that the superconductivity is destroyed in the vortex core. Since the healing length of the order parameter is the coherence length, this means the core should be roughly size ξ. Thus the energy per unit length of the core is the condensation energy denisty $H_c^2/(2\mu_0)$ times the area of the vortex core, $\pi\xi^2$. We thus have

$$\frac{\text{Energy}}{\text{Length}} = \epsilon = \frac{H_c^2}{2\mu_0}\pi\xi^2 \approx \frac{H_c^2}{\mu_0}\xi^2$$

where here we are dropping order unity factors (since we are not going to get them right anyway!). We thus have

$$H_{c1} = \frac{\epsilon}{2\phi_0} \approx \frac{\mu_0 H_c^2 \xi^2}{\phi_0} \approx \frac{\phi_0}{\lambda^2}\frac{1}{\mu_0} \tag{6.19}$$

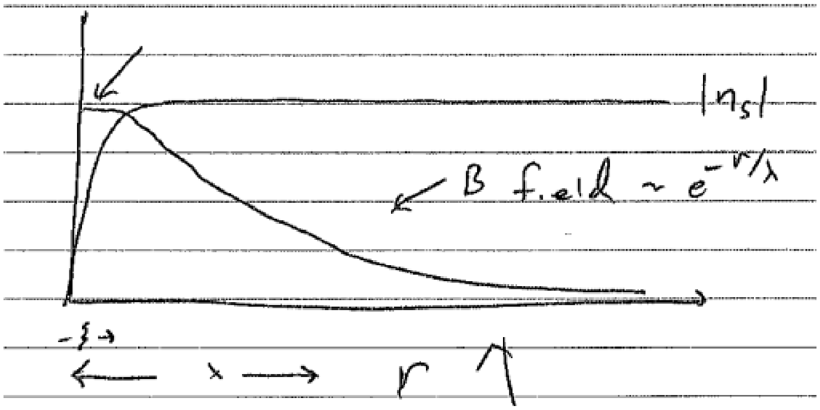

Figure 6.6: The order parameter heals over a short length scale ξ whereas the magnetic field is screened over a longer scale λ.

where we are again dropping order one factors and in the last step we have used the expression Eq. 6.18 for H_c. The meaning of this result is that H_{c1}, the lowest field where a vortex can penetrate a superconductor, is given by the magnetic field necessary such that a single flux quantum penetrates a square area of size λ by λ, as shown in the right of Fig. 6.5.

Comparing Eq. 6.18 to 6.19 we see that in order for H_{c1} to be less than H_c we must have

$$\frac{\lambda}{\xi} \gtrsim 1$$

which should be the necessary condition for a Type II superconductor. (We have dropped constants of order unity, so we should not expect to get the precise value correct.)

Conventionally one defines the dimensionless ratio known as the Ginzburg-Landau parameter

$$\kappa = \frac{\lambda(T)}{\xi(T)} = 2\sqrt{\frac{\alpha_4}{\mu_0}}\;\frac{m^*}{\hbar e^*}$$

which is temperature independent (at least whenever Ginzburg-Landau theory is valid).

A more precise calculation can be done to give the condition for a Type II superconductor is that $\kappa > \frac{1}{\sqrt{2}}$.

In order to have a vortex we must have a type II superconductor, meaning, $\kappa \gtrsim 1$. This means the London penetration depth, the screening length for magnetic fields, is longer than the coherence length, the healing length for the order parameter. Thus around a vortex core, the order parameter heals quickly whereas the magnetic field is screened slowly. This is roughly depicted in Fig. 6.6.

In fact a more precise calculation will show that the energy of an isolated vortex will have a $\log\kappa$ correction that we ignored. By calculating the energy of the vortex core, we found that the energy per unit length is (See Eq. 6.19)

$$\epsilon \approx 2\mu_0 H_c^2 \xi^2$$

However, the actual result includes a term of the form

$$\mu_0 H_c^2 \xi^2 \log(\lambda/\xi)$$

To understand where this term comes from, we roughly say that at radius less than λ we can neglect the screening due to the electromagnetism and the order parameter around the vortex core will be similar to what it is for a neutral superfluid. In this case, the order parameter is $\psi \sim e^{i\theta}$ so there is a velocity $v \sim \nabla\theta \sim 1/r$ in the $\hat{\theta}$ direction. The Ginzburg-Landau kinetic energy density will give us something of the form

$$KE = \frac{mv^2}{2} \sim \frac{1}{r^2}$$

we then have a total energy

$$E \sim \int d^2r \frac{1}{r^2} \sim \int_\xi^\lambda dr \frac{1}{r} \sim \log(\lambda/\xi)$$

where we have cut off the integral at ξ because below this, the order parameter drops and we also cut off at λ because above this radius the screening makes the current drop exponentially.

Chapter 7

Interacting Fermions

7.1 Why study fermions

Having spent the entire course so far discussing bosons, we now turn our attention to fermions, and interacting fermions in particular.

Why should we study interacting fermions? There are several **good reasons** for this

Electrons (which are fermions) are the world[1]. The physics of every metal, every semiconductor, every insulator, is completely controlled by the behavior of its electrons. In fact essentially all of chemistry is nothing more than the study of the behavior of electrons in different environments.

Usually when a condensed matter physicist says they are studying fermions, they mean they are studying electrons. There is one notable exception[2] to this: the fermion ^{3}He. This fermionic isotope[3] of Helium is a favorite of condensed matter. As with the bosonic version, the light mass of Helium prevents it from forming a solid at low temperatures, and instead we get a quantum fluid — or Fermi liquid. However, as compared to electrons, it has short range interactions rather than long range Coulomb interactions, and this makes its physics somewhat simpler in many ways[4]. An enormous amount has been learned from

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[1] You can imagine all the electrons getting together and holding hands and singing "We are the world...!". At this point, anyone reading this footnote probably thinks I have gone crazy, but I've been typing these notes for a lot of hours in a row, and yes, maybe I'm going a bit batty.

[2] In the modern era of cold atomic gases, there are now experiments on fermionic cold atoms too.

[3] Helium-3 (^{3}He) was discovered experimentally in 1934 by Mark Oliphant at Cambridge. A mere few milligrams of the material became available for experiments as an offshoot of the post-war nuclear program. Now it is much more plentiful due to the fact that it is a waste product of nuclear missiles (Tritium, a fuel of hydrogen bombs, has a half-life of 12 years, and decays into ^{3}He). The price of Helium 3 fluctuates between 100 and 10000 dollars per litre, depending on the global supply at the time.

[4] One interesting feature we will not discuss in depth is that at extremely low temperaturures (meaning sub milli Kelvin) ^{3}He actually becomes a superfluid. The experimental discovery of this in 1972 earned Lee, Osheroff and Richardson a Nobel prize in 1996. Theoretical work on the subject earned a Nobel prize

the study of this fermion. We will return to discussion of this below in section 9.1.

We need to understand strongly interacting fermions. In all of our introductory courses on solid state physics, we learn about metals, semiconductors, and insulators completely ignoring the interactions between electrons. But in fact in typical materials, the interaction energy is on the order of the kinetic energy, or even larger. It seems crazy to have ignored it! So why on earth is it OK for us to ignore interactions altogether in these simple pictures. At some level the interactions must have some effect — what are these effects?

Eventually we want to study superconductivity!. We have so far treated superconductivity crudely as simply thinking about bosons with charge $e* = 2e$, but this is completely wrong for a number of reasons:

- Electrons repel each other *very* strongly. It seems crazy to think of them forming pairs[6].

- Even if you could manufacture some weak attraction between fermions, to make a true boson that you could condense, you would need a binding radius smaller than the inter-electron distance. This would require a binding energy on the order of the Fermi energy, which is huge![7]

7.2 Some Mathematical Preliminaries Regarding Fermions

Although it is possible to do almost every calculation in first quantized notation, it becomes rapidly extremely messy to do so. It is really better to just bite the proverbial bullett and introduce second quantization and then talk in that language. The preliminaries introduced here are the fermionic analogs of the preliminaries introduced in section 4.1 for bosons.

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for Tony Leggett[5] in 2003. Similar to electons pairing at low temperature to superconduct, Helium 3 forms pairs at low tempertaure in order to form a superfluid.

[5] See also comment about Leggett's opinion of number non-conserving order parameters in section 4.4. Tony Leggett was an undergraduate at Oxford, *in Classics!*. (More properly the degree was called "greats" or something like that at the time). After his undergrad degree he managed to convince a tutor to let him study physics, which he says he struggled with at first. In his Nobel biography he tells an entertaining story about rowing in his first year at Oxford (since everyone was doing it) and feeling like he was actually doing well, until they swapped him for the coxswain.

[6] Landau famously said "You cannot repeal Coulomb's law!"

[7] This very strong binding is precisely what happens to create the boson ^{4}He out of two neutrons, two protons, and two electrons. However, with electrons interacting with other electrons, there is no analogous strong attraction mechanism.

7.2.1 Second Quantization

Orthonormal Single Particle Basis

Suppose we have a set of orthonormal orbitals which we will label $i, j, k, \ldots$. What we mean by this is wavefunctions $\varphi_i(\mathbf{r}, \sigma), \varphi_j(\mathbf{r}, \sigma), \varphi_k(\mathbf{r}, \sigma), \ldots$. Here note that the wavefunction is a function of both position and particle spin. The orthonormality condition is[8]

$$\langle i|j\rangle = \sum_\sigma \int d\mathbf{r}\; \varphi_i^*(\mathbf{r},\sigma)\varphi_j(\mathbf{r},\sigma)$$

we will frequently abbreviate this kind of integral as

$$\langle i|j\rangle = \int d(1)\; \varphi_i^*(1)\varphi_j(1)$$

where here (1) is meant to indicate positions and spins (if we have particles with spin).

Many-Fermion Slater Determinant

A many-body fermionic wavefunction must be fully antisymmetric. We can write down a convenient basis of fully antisymmetric states using so-called *Slater* determinants[9]. We write

$$\Psi(\tilde{1}, \tilde{2}, \ldots, \tilde{M}) = \frac{1}{\sqrt{M!}} \begin{vmatrix} \varphi_1(\tilde{1}) & \varphi_1(\tilde{2}) & \ldots & \varphi_1(\tilde{M}) \\ \varphi_2(\tilde{1}) & \varphi_2(\tilde{2}) & \ldots & \varphi_2(\tilde{M}) \\ \vdots & \vdots & & \vdots \\ \varphi_M(\tilde{1}) & \varphi_M(\tilde{2}) & \ldots & \varphi_M(\tilde{M}) \end{vmatrix}$$

Here for clarity, the numbers with tildes over them $\tilde{1}, \tilde{2}, \ldots$ are the position and spin variables, whereas the subscripts $_{1}, _{2}, \ldots$ are orbital indices. If the constituent orbitals are orthonormal then the Slater determinants are properly normalized

$$\langle \Psi|\Psi\rangle = \int d(\tilde{1})d(\tilde{2})\ldots d(\tilde{M})\Psi^*(\tilde{1}, \tilde{2}, \ldots, \tilde{M})\; \Psi(\tilde{1}, \tilde{2}, \ldots, \tilde{M}) = 1 \tag{7.1}$$

where again the integrals $d(\tilde{1})$ means both to integrate over space and sum over spin. Further, two Slater determinants made from different sets of orthonormal orbitals will be orthogonal.

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[8] The observant reader will realize this is nothing more than a completeness relationship

$$\langle i|j\rangle = \sum_x \langle i|x\rangle\langle x|j\rangle$$

where x is the position and spin basis.

[9] Slater was a professor at MIT for many years.

Fermionic Creation Operators

We define a set of Fermionic creation operators $c_i^\dagger$ corresponding to the orbitals φ_i. These operators are defined by the following statement: Applying creation operators to the vacuum gives a Slater determinant of the corresponding orbitals. In particular

$$c_1^\dagger c_2^\dagger \ldots c_M^\dagger |0\rangle = \frac{1}{\sqrt{M!}} \begin{vmatrix} \varphi_1(\tilde{1}) & \varphi_1(\tilde{2}) & \ldots & \varphi_1(\tilde{M}) \\ \varphi_2(\tilde{1}) & \varphi_2(\tilde{2}) & \ldots & \varphi_2(\tilde{M}) \\ \vdots & \vdots & & \vdots \\ \varphi_M(\tilde{1}) & \varphi_M(\tilde{2}) & \ldots & \varphi_M(\tilde{M}) \end{vmatrix}$$

Let us look at the normalization condition Eq. 7.1. In terms of these operators we have

$$1 = \langle \Psi | \Psi \rangle = \langle 0 | c_M \ldots c_1 \;\, c_1^\dagger \ldots c_M^\dagger | 0 \rangle \tag{7.2}$$

We should thus think of $c_i^\dagger$ as an operator that adds a fermion to orbital i, and correspondingly c_i is an operator that removes a fermion from orbital i. So in Eq. 7.2 we start on the far right with the vacuum, we add a fermion in orbital M and then in $M-1$ and so forth until we add a fermion in orbital 1, then continuing towards the left we remove the fermions in the opposite order until we are back to the vacuum. Alternately we can think of the c_i operators as just being creation operators that have been hermitian conjugated so that they act on the dual space to the left. I.e., $\langle 0 | c_i$ is the dual (hermitian conjugate) to the wavefunction $c_i^\dagger |0\rangle$, and both represent one particle created in an orbital.

Anticommutations

Note that the fermionic creation operators must anticommute

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger$$

This is because if we switch the order of creation of two orbitals, this corresponds to switching two rows of the Slater determinant — which incurs a minus sign. Similarly, we can conclude

$$c_i c_j = -c_j c_i$$

Further, we have

$$c_i^\dagger c_i^\dagger = 0$$

since you cannot put two fermions in the same orbital (or equivalently, if two rows of a Slater determinant are the same, the determinant vanishes). Similarly we have the dual statement

$$c_i c_i = 0$$

meaning that you can only annihilate a particle, at most, once.

Finally we note that

$$c_i^\dagger c_i + c_i c_i^\dagger = 1 \tag{7.3}$$

To see this is true we apply this expression to an arbitrary $|\text{state}\rangle$. We can decompose the $|\text{state}\rangle$, into two parts, one in which orbital i is filled and one in which orbital i is empty (there are no other possibilities for fermions). If the orbital is filled then

$$c_i^\dagger c_i |\text{state}\rangle = |\text{state}\rangle$$

since the fermion in orbital i is removed and then put back. On the other hand

$$c_i c_i^\dagger |\text{state}\rangle = 0$$

since it is trying to create another fermion in orbital i which is already filled.

On the other hand, if orbital i is empty we have

$$c_i c_i^\dagger |\text{state}\rangle = |\text{state}\rangle$$

since we can add a particle to orbital i then remove it again. And also we have

$$c_i^\dagger c_i |\text{state}\rangle = 0$$

since we are trying to annihilate a particle from an orbital that is already empty. Putting these statements together we find that Eq. 7.3 is satisfied independent of whether it acts on a filled or empty orbital.

We can summarize many of these results by defining anticommutator brackets. For any operators let us define

$$\{A, B\} = AB + BA$$

All of the previous results in this subsection are summarized with the following statements[10]:

$$\begin{aligned} \{c_i, c_j\} &= \{c_i^\dagger, c_j^\dagger\} = 0 \qquad (7.4) \\ \{c_i, c_j^\dagger\} &= \delta_{ij} \qquad (7.5) \end{aligned}$$

7.2.2 Change of Basis

As in the bosonic case we can consider changing the basis for our orbitals. Let us suppose we have two sets of orthonormal basis orbitals. One set we call $\{|\alpha\rangle\}$ and the other set

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[10] The observant reader will notice that in fact we have not yet shown Eq. 7.5 for $i \neq j$. This is required by consistency. To see this let us try writing (with $i \neq j$)

$$c_j^\dagger |0\rangle = c_j^\dagger c_i c_i^\dagger |0\rangle$$

But also

$$c_j^\dagger |0\rangle = c_i c_i^\dagger c_j^\dagger |0\rangle = -c_i c_j^\dagger c_i^\dagger |0\rangle$$

Since these two lines must equal each other, we must have $c_j^\dagger c_i = -c_i c_j^\dagger$

we call $\{|i\rangle\}$. We can derive creation operators in a new basis in terms of the creation operators in the old basis (this is entirely analogous to Eq. 4.5 for bosons)

$$c^\dagger_\alpha = \sum_i \langle i|\alpha\rangle c^\dagger_i$$

A useful example of such a basis change is from tight binding orbitals to plane waves on a lattice (where we leave the spin unchanged in this particular case).

$$c^\dagger_{\mathbf{r};\sigma} = \sum_{\mathbf{k}} \langle \mathbf{k},\sigma|\mathbf{r},\sigma\rangle c^\dagger_{\mathbf{k};\sigma} = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} c^\dagger_{\mathbf{k};\sigma}$$

Often we would like to use continuum fields $\mathbf{r}$ rather than lattice points, in which case we write $\hat{\psi}^\dagger_\sigma(\mathbf{r})$ instead of $c^\dagger_\sigma(\mathbf{r})$. In this case the fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ obey the anticommutations

$$\{\hat{\psi}^\dagger_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')\} = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}$$

If we have an orbital basis $\varphi_i(\mathbf{r},\sigma)$ we can write the creation operators in this basis in terms of the $\hat{\psi}$ operators as

$$\begin{aligned} c^\dagger_i &= \sum_\sigma \int d\mathbf{r}\, \varphi_i(\mathbf{r},\sigma)\hat{\psi}_\sigma(\mathbf{r}) \\ &= \int d(1)\varphi_i(1)\hat{\psi}^\dagger(1) \end{aligned}$$

Important Example: Fermi Sea As an example, let us consider a sytem of $\mathbf{k}$ states filling a Fermi sea. We can write

$$|\text{Fermi Sea}\rangle = \prod_{|\mathbf{k}|<k_f} \prod_{\sigma=\uparrow,\downarrow} c^\dagger_{\mathbf{k},\sigma}|0\rangle \tag{7.6}$$

We note that there is some presumed fiducial[11] ordering of operators in these products. Without an ordering we cannot establish the sign of the wavefunction. Fortunately, we may never need to actually specify the ordering, but we should be very careful to keep track of any changes to the ordering, since any exchange incurs a minus sign.

7.2.3 Writing our Hamiltonian in Second Quantized Form

We will typically be concerned with a Hamiltonian of the form

$$H = H_0 + H_{int}$$

where[12]

$$H_0 = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i)\right] = \sum_i \hat{h}_i$$

---

[11] Fiducial means essentially "accepted as a fixed reference".

[12] I apologize that here I've used U for single particle potential and V for interaction, whereas in prior sections it was the other way around. I hope this does not create too much confusion!

is the single particle Hamiltonian of particles in a trapping potential $U(\mathbf{r})$ and

$$H_{int} = \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j)$$

is the interaction between particles. This might be, for example, a Coulomb interaction if we are considering electrons.

We now want to rewrite these in second quantized form.

To do this we can write the particle density,

$$\rho(\mathbf{r}) = \sum_{\sigma} \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r})$$

so that we can write the interaction as

$$\begin{aligned} H_{int} &= \frac{1}{2} \int d(1) \int d(2) : \rho(1)\, V(1-2)\, \rho(2) : \\ &= \frac{1}{2} \int d(1) \int d(2) : \hat{\psi}^{\dagger}(1)\hat{\psi}(1)\ V(1-2)\ \hat{\psi}^{\dagger}(2)\hat{\psi}(2) : \end{aligned}$$

As in section 4.3 we have added colons : to indicate that the expression should be normal ordered which implies we should move all the creation operators to the left (and remember to add a minus sign for each exchange). To justify this we consider a system with a single fermion — without the normal ordering colons, this single fermion would have a nonzero self-interaction.

We can thus rewrite the interaction term as

$$H_{int} = \frac{1}{2} \int d(1) \int d(2) \hat{\psi}^{\dagger}(1)\hat{\psi}^{\dagger}(2)\ V(1-2)\ \hat{\psi}(2)\hat{\psi}(1) \tag{7.7}$$

The single particle term, we can write as

$$H_0 = \int d(1)\ \hat{\psi}^{\dagger}(1) \left[\frac{-\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) \right] \hat{\psi}(1) \tag{7.8}$$

To see that this is correct, we rewrite $\psi^{\dagger}$ in terms of some single particle basis $|\alpha\rangle$.

$$\hat{\psi}^{\dagger}(1) = \sum_{\alpha} \varphi^*_{\alpha}(1) c^{\dagger}_{\alpha}$$

so that we have

$$H_0 = \sum_{\alpha,\beta} h_{\alpha\beta} c^{\dagger}_{\alpha} c_{\beta} \tag{7.9}$$

where

$$h_{\alpha,\beta} = \langle \alpha | \hat{h} | \beta \rangle = \int d(1)\ \varphi^*_{\alpha}(1) \left[\frac{-\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) \right] \varphi_{\beta}(1)$$

It is most convenient at this point (although certainly not necessary) to choose a basis $|a\rangle$ that are eigenvectors of the operator $\hat{h}$ with eigenvalues ϵ_a^0, so we have

$$\hat{h}|a\rangle = \epsilon_a^0|a\rangle$$

Thus we can write

$$H_0 = \sum_a \epsilon_a^0 \; c_a^\dagger c_a \tag{7.10}$$

The meaning of this expression is quite clear. The operators $\hat{n}_a = c_a^\dagger c_a$ counts the number of fermions (0 or 1) in orbital a, and if there is a fermion in the orbital, it is assigned an energy ϵ_a^0.

It is then useful to write the interaction part of the Hamiltonian Eq. 7.8 in an orbital basis to obtain

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \; c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \tag{7.11}$$

where the matrix element $v_{\alpha\beta\gamma\delta}$ is given by

$$v_{\alpha,\beta,\gamma,\delta} = \langle\alpha\beta|V|\gamma\delta\rangle = \int d(1) \int d(2) \; \varphi_\alpha^*(1)\varphi_\beta^*(2)\, V(1-2)\, \varphi_\gamma(1)\varphi_\delta(2) \tag{7.12}$$

Note carefully the ordering of the indices in Eq. 7.11 (the last two indices in the two sets of subscript are switched). To see where this comes from compare Eq. 7.7 to Eq. 7.12. We will continue to use this convention, although other conventions are possible as well.

Obviously the matrix element $\langle\alpha\beta|V|\gamma\delta\rangle$ in Eq. 7.12 uses a two-particle basis

$$|\gamma\delta\rangle \rightarrow \varphi_\gamma(1)\varphi_\delta(2)$$

which is not properly symmetrized for fermions. The symmetrization is automatic though once we put these matrix elements into Eq. 7.11 using the fermionic creation operators.

Note also that the matrix element has a number of obvious symmetries including

$$v_{\alpha\beta\gamma\delta} = v_{\beta\alpha\delta\gamma} \tag{7.13}$$

The Hamiltonian $H = H_0 + H_{int}$ with H_{int} written in the form of Eq. 7.11 and H_0 written in the form of Eq. 7.9 or Eq. 7.14 will be our object of study for the rest of this chapter. This form is extremely general and can be used for study of any interacting Fermi system, such as electrons in a metal, electrons in an atom, Helium 3, or even neutrons in a neutron star.

We will use several different "first pass" approximations (first order perturbation theory, Hartree approximation, Hartree-Fock, etc). Sometimes these approximations will give the same results, but sometimes they will not.

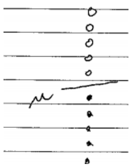

Figure 7.1: (Ignore the lined paper!). This depicts filling all orbitals up to the chemical potential.

7.3 First Order Perturbation Theory

Let us work in a basis such that the single particle Hamiltonian H_0 is diagonal. We thus have

$$H_0 = \sum_a \epsilon_a^0 \; c_a^\dagger c_a \tag{7.14}$$

Ignoring the interaction ("zeroth" order in interaction) the ground state is just to fill up all orbitals below the chemical potential μ.

$$|\text{Noninteracting Ground State}\rangle = |\text{GS}^0\rangle = \left[\prod_{a \text{ occupied}} c_a^\dagger \right] |0\rangle \tag{7.15}$$

where here an orbital a is occupied if

$$\epsilon_a^0 < \mu$$

as depicted schematically in Fig.7.1. As in Eq. 7.6, there is some presumed ordering of orbitals in Eq. 7.15 which we will not specify.

Next we want to include the interaction term. We write this term as above in the form (Same as Eq. 7.11)

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \; c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \tag{7.16}$$

At first order in perturbation theory the correction to the energy is

$$\delta E = \langle \text{GS}^0 | H_{int} | \text{GS}^0 \rangle$$

We now have to evaluate this expectation. We could do this by commuting a bunch of operators around, but there is a simple "shortcut" way of thinking:

$$\delta E = \underbrace{\langle 0| \prod_{e \text{ occupied}} c_e \;|}_{\text{same filled state}} \; \frac{1}{2}\sum_{abcd} v_{abcd} \;\; \underbrace{c_a^\dagger c_b^\dagger}_{\text{return same two}} \;\; \underbrace{c_d c_c}_{\text{remove two}} \;\; \underbrace{| \prod_{f \text{ occupied}} c_f^\dagger \, |0\rangle}_{\text{1filled state}}$$

Here we note that the initial ket and final bra are exactly the same state. This means whichever particles are removed by $c_d c_c$ have to be returned by $c_a^\dagger c_b^\dagger$. There are exactly two ways in which this can happen: Either a matches c and b matches d,

$$\contraction{}{c_a^\dagger}{\, c_b^\dagger \, c_d \,}{c_c} \contraction[2ex]{c_a^\dagger \,}{c_b^\dagger}{\,}{c_d} c_a^\dagger \, c_b^\dagger \, c_d \, c_c$$

or a matches d and b matches c

$$c_a^\dagger \, c_b^\dagger \, c_d \, c_c$$

We thus obtain

$$\delta E = \langle H_{int} \rangle = \frac{1}{2} \sum_{a,b \text{ occupied}} (v_{abab} - v_{abba}) \tag{7.17}$$

It is clear that the two terms should have opposite signs since one commutation will make them look the same. To be more precise about the signs, note that in the first case (were a matches c) we can write the contribution as

$$\langle 0| \prod_{e \text{ occupied}} c_e \;|\; c_a^\dagger c_b^\dagger \quad c_b c_a \;|\; \prod_{f \text{ occupied}} c_f^\dagger \, |0\rangle = \langle \text{state}|\text{state}\rangle$$

so we end up with a positive sign. On the other hand, to get the second case into this form we need to anticommute two of the operators and thus pick up an minus sign.

This approach, can at least in principle, be extended systematically to higher order perturbation theory.

7.3.1 Hartree and Fock Terms

The two terms in Eq. 7.17 have different meanings. Let us study them one at a time.

Hartree, or Direct, Term

Using Eq. 7.12 the first term in Eq. 7.17 is given by

$$v_{abab} = \int d(1) \int d(2) |\varphi_a(1)|^2 |\varphi_b(2)|^2 V(1-2) \tag{7.18}$$

This is known as the Hartree[13] or Direct interaction term. This is simply the interaction of the density in orbital a with the density in orbital b. If we keep only this term in Eq. 7.17 we have what is known as the Hartree approximation, which is somewhat simpler than the full first order perturbation calculation.

Self-Consistent Hartree We can also consider doing a self-consistent version of this calculation. This is a common approach known as *self-consistent Hartree.* It amounts to solving the Schroenger equation in a potential which includes the interaction from all the other electrons in the system[14]. In other words we write

$$\begin{aligned} U^{eff}(\mathbf{r}) &= U(\mathbf{r}) + \int d\mathbf{r}' \sum_{n \text{ occupied}} |\varphi_n(\mathbf{r}')|^2 V(\mathbf{r}-\mathbf{r}') \\ &= U(\mathbf{r}) + \int d\mathbf{r}' \; \langle \rho(\mathbf{r}') \rangle \; V(\mathbf{r}-\mathbf{r}') \end{aligned}$$

---

[13] Douglas Hartree was a British Numerical expert. He has a unit, the Hartree, named after him (which is $e^2/(4\pi\epsilon_0 a_0) = 2\text{Ry} \approx 27.2\text{eV}$).

[14] Self-consistent Hartree for bosons is precisely the Gross-Pitaevskii equation! See discussion near Eq.4.13.

The procedure for implementing self-consistent Hartree is as follows:

1. Solve the Schroedinger equation in the presence of the potential $U^{eff}(\mathbf{r})$
2. Fill the lowest N orbitals, and calculate $\langle\rho(\mathbf{r})\rangle$
3. Recalculate U^{eff}
4. Go back to step 1, and repeat until converged.

Fock, or Exchange, Term

Using Eq. 7.12 the second term in Eq. 7.17 is given by

$$v_{abba} = \int d(1) \int d(2)\; \varphi_a^*(1)\varphi_b^*(2)\, V(1-2)\, \varphi_b(1)\varphi_a(2) \tag{7.19}$$

Note in particular that this term is zero unless the orbitals a and b overlap[15]. Note in particular that this means that orbital a and b need to overlap both in space *and* in spin space[16]. Eq. 7.19 is known as the Fock[17] or exchange term. This term cannot be described as simply some sort of effective potential that an electron moves in, as the Hartree term was. Note also that if the potential $V(r)$ is repulsive, the Fock term (which enters in Eq. 7.17 with a minus sign) is attractive.

Further Comments on First Order Perturbation Theory

It should be noted that, despite the fact that we have a Hartree term and a Fock term, what we have calculated so far (Eq. 7.17) is NOT the Hartree-Fock approximation (admittedly the nominclature is confusing).

We should also note that first order perturbation theory can also be used to (approximately) calculate the energy shift, due to interactions, of excited states. Again, if we

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[15] If the *support* of φ_a and φ_b (meaning the region where they are nonzero) is disjoint then there is no value of the variable 1 for which the integrand is nonzero

[16] For example, since

$$\int d(1)\varphi_a^*(1)\varphi_b(1) = \int d\mathbf{r} \sum_\sigma \varphi_a^*(\mathbf{r},\sigma)\varphi_b(\mathbf{r},\sigma)$$

If we work with orbitals having a definite spin, the two orbitals would have to have the same spin for this to be nonzero.

[17] Vladimir Fock was the creator of the idea of second quantization in 1932 (although some of the ideas were presented by Dirac as early as 1927). Fock is immortalized through the idea of "Fock space". Much of Fock's later career was devoted to philosophy of science. He became a defender of relativity in a hostile Marxist world. Unfortunately, some of the Marxist philosophers thought that modern physics was "Bourgeois" and therefore dangerous to the state. Fock was forced to become a philosopher, speak their language, and clarify what is physics and what is philosophy. It is unclear how well Soviet physics would have survived were it not for Fock.

begin with the noninteracting system, we can write an excited state as

$$|\text{Excited}\rangle = c_j^\dagger c_i |\text{GS}^0\rangle$$

where i is one of the orbitals which is filled in the noninteracting ground state, and j is one of the orbitals which is empty in the noninteracting ground state. Without interactions the energy of this excited state is

$$E^0_{excited} = \epsilon^0_j - \epsilon^0_i + E^0_{groundstate}$$

Again we can calculate the energy shift due to interactions as

$$\delta E = \langle H_{int} \rangle = \frac{1}{2} \sum_{a,b \text{ occupied}} (v_{abab} - v_{abba})$$

with the expectation given in the excited state, meaning that the sum over occupied states includes orbital j but not orbital i.

7.4 Hartree-Fock Approximation

The so-called Hartree-Fock approximation is a self-consistent mean-field theory approach. It is often the first approach a theorists tries, and it is used extensively in condensed matter physics, but also in nuclear physics, atomic physics, molecular chemistry[18], and so forth.

Let us briefly recall the (Weiss) mean field method for understanding ferromagnets. Here we have a Hamiltonian like the Heisenberg Hamiltonian

$$H = \frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where, for example, the sum is over neighboring spins i, j. To handle this interaction we average one of the spins and leave the other one un-averaged,. So we have instead a Hamiltonian for a single spin given by

$$h_j = J \sum_{j \text{ neighbors } i} \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle$$

with $\langle \mathbf{S}_j \rangle = \langle \mathbf{S} \rangle$ is the average of the spin on any site. We can then solve the single site problem, and we need to "self-consist" meaning that the solution of the single-site problem should give us $\langle \mathbf{S} \rangle$.

We hope to use the same mean-field idea to handle the interaction term of our Hamiltonian. We thus take

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \; c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \tag{7.20}$$

---

[18] A Nobel Prize in chemistry was awarded to John Pople in 1998 for developing numerical Hartree Fock methods for simulating molecules.

and we replace it with

$$H^{eff}_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \left[\langle c^\dagger_\alpha c_\gamma \rangle c^\dagger_\beta c_\delta + \langle c^\dagger_\beta c_\delta \rangle c^\dagger_\alpha c_\gamma - \langle c^\dagger_\alpha c_\delta \rangle c^\dagger_\beta c_\gamma - \langle c^\dagger_\beta c_\gamma \rangle c^\dagger_\alpha c_\delta \right] \tag{7.21}$$

Here we have taken all possible (nonzero) averages of two operators and left two other operators unaveraged[19] Note also that due to the symmetry Eq. 7.13 the first two terms in the square brackets are identitical to each other and the last two terms are also identical to each other.

We can thus write a more abbreviated form

$$H^{eff}_{int} = \sum_{\alpha,\delta} f_{\alpha\delta} \; c^\dagger_\alpha c_\delta \tag{7.22}$$

where

$$f_{\alpha\delta} = \sum_{\beta,\gamma} \langle c^\dagger_\beta c_\gamma \rangle \left[v_{\alpha\beta\delta\gamma} - v_{\alpha\beta\gamma\delta} \right] \tag{7.23}$$

Including the single-body terms $h_{\alpha\beta}$ (See Eq. 7.9) we have

$$H^{eff} = \sum_{\alpha\delta} \left[h_{\alpha\delta} + f_{\alpha\delta} \right] \; c^\dagger_\alpha c_\delta \tag{7.24}$$

The two equations Eq. 7.23 and 7.24 constitute the Hartree-Fock approximation. Our procudure for solving these two equations at the same time is iterative (similar to the above described, self-consistent Hartree approach). While in principle one can produce a solution in any basis, it is convenient to successively change basis as we iterate to convergence. We thus follow the following procedure

1. Let ϵ_μ be the eigenvalues of $h_{\alpha\delta} + f_{\alpha\delta}$ with corresponding eigenvectors $|\mu\rangle$.
2. Change to this eigenbasis by defining

   $$\tilde{c}^\dagger_\mu = \sum_\alpha \langle \alpha | \mu \rangle c^\dagger_\alpha$$

   In this basis, the Hamiltonian is of the form

   $$H^{eff} = \sum_\mu \epsilon_\mu \tilde{c}^\dagger_\mu \tilde{c}_\mu$$

3. Fill the lowest N states with our fermions (Assuming we have an N fermion system)

   $$|\Psi\rangle \prod_{\text{lowest } N} \tilde{c}^\dagger_\mu |0\rangle$$

---

[19] When we get to superconductivity, we will also consider the possibility of needing terms like $\langle c^\dagger c^\dagger \rangle$ and $\langle cc \rangle$. However if we insist on a system with a definite number of particles, such expectations are strictly zero.

4. Recalculate $f_{\alpha\delta}$ in this new ground state using Eq. 7.23. Note that this recalculation is why we wanted to work in the diagonal basis. In this basis we have

$$\langle c^\dagger_\mu c_\nu \rangle = \delta_{\mu\nu} \times \begin{cases} 1 & \text{if } \mu \text{ is filled} \\ 0 & \text{if } \mu \text{ is empty} \end{cases}$$

   We thus have

$$f_{\alpha\delta} = \sum_{\mu \text{ occupied}} [v_{\alpha\mu\delta\mu} - v_{\alpha\mu\mu\delta}] \tag{7.25}$$

5. Go back to step 1 and repeat until convergence. When it converges, the old basis and the new basis match. This means, that in this basis, $h + f$ is already diagonal. Thus we have

$$\epsilon_\mu = h_{\mu\mu} + f_{\mu\mu} = h_{\mu\mu} + \sum_{\nu \text{ occupied}} [v_{\mu\nu\mu\nu} - v_{\mu\nu\nu\mu}]$$

   The first term in the square brackets being from the Hartree term and the second term being from the Fock term.

Note that if we were to follow exactly the same procedure, but using only the first (Hartree) of the two v terms, we would have the self-consistent Hartree approximation, as described above.

The energies ϵ_μ can be thought of as the Hartree-Fock ionization energies. I.e., this is the energy (in Hartree-Fock approximation) required to remove the electron in the μ orbital. This results is known as Koopmans' theorem[20]. The total energy of the Hartree-Fock system is given by

$$E_{total} = \sum_{\mu \text{ filled}} \left[h_{\mu\mu} + \frac{1}{2} f_{\mu\mu} \right] \tag{7.26}$$

The factor of 1/2 here is similar to what occurs in Weiss mean field theory. In writing down the total energy of the system, one does not want to overcount the energy of spin i interacting with spin j and also spin j interacting with spin i. It is quite similar here. Simple addition of all of the ϵ_μ Hartree Fock ionization energies would count interaction of each particle μ with all the other particles ν but then would again count the interaction of each ν with μ. Thus we need to introduce the factor of 1/2 in the interaction.

---

[20] Tjalling Koopmans is a Nobel laureate in the field of economics (never mind that economics was not one of the original subjects that Nobel had established prizes for — so it is strictly speaking a Nobel memorial medal, not a Nobel prize). He did his work on Hartree-Fock in 1934 when he was a 24 year old grad student, but shortly thereafter switched fields to economics. His prize in 1975 was awared for the theory of optimal allocation of resources. Apparently his own resource was more optimally allocated in the field of economics. The word "Koopman" in dutch means "Trader" or "Merchant", possibly justifying his attraction to the field of economics.

7.4.1 Hartree-Fock as Optimal Slater Determinant

We claim that the solution of the Hartree-Fock equations provides the best (lowest energy) variational wavefunction in the form of a single Slater determinant. This optimal wavefunction is

$$|\mathrm{HF}\rangle = \prod_{\mu \text{ filled}} c^\dagger_\mu |0\rangle$$

for the Hartree-Fock orbitals μ. This brings us to an equivalent definition of the Hartree-Fock approximation:

Hartree-Fock is an approximation by which one finds the optimal ground state wavefunction in the form of a single Slater determinant.

Proof that this statement is equivalent to the Hartree-Fock equations derived as a mean field theory above (Eq. 7.23 and 7.24) is nontrivial. We will present it here.

Proof:

Consider a basis of orbitals μ and a single Slater determinant (or "filled Fermi sea") made of these orbitals.

$$|\mathrm{GS}\rangle = \prod_{\mu \, \text{filled}} c^\dagger_\mu |0\rangle$$

We would like to find a condition such that $|\mathrm{GS}\rangle$ is a variational minimum. To find this condition we want to try varying the basis μ and seeing if the energy decreases. So let us imagine switching to a new basis

$$\tilde{c}^\dagger_\alpha = \sum_\mu \langle \mu | \alpha \rangle c^\dagger_\mu = \sum_\mu U_{\alpha\mu} c^\dagger_\mu \tag{7.27}$$

where U is a unitary matrix. Note that we are only concerned with a change of basis which mixes filled and empty orbitals. If we change basis in a way that that mixes two filled orbitals with each other, or in a way that mixes two empty orbitals with each other, the resulting Slater determinant remains unchanged[21,22]. At the same time we want the

---

[21] Let us see an example of this. Suppose we make the basis transform

$$\begin{aligned} \tilde{c}^\dagger_a &= (c^\dagger_1 + c^\dagger_2)/\sqrt{2} \\ \tilde{c}^\dagger_b &= (c^\dagger_1 - c^\dagger_2)/\sqrt{2} \end{aligned}$$

It is easy to check that if both orbitals are filled, the basis change does not change the resulting Slater determinant:

$$\tilde{c}^\dagger_a \tilde{c}^\dagger_b |0\rangle = c^\dagger_1 c^\dagger_2 |0\rangle$$

However if we only fill one of these two orbitals

$$\tilde{c}^\dagger_a |0\rangle \neq c^\dagger_1 |0\rangle \neq c^\dagger_2 |0\rangle$$

Thus to change the Slater determinant, we need to mix a filled state with an empty state.

[22] We should be cautious that rewriting a determinant of orbitals in terms of an equivalent set of orbitals can sometimes incur an overall sign to the wavefunction if we somehow reorder the orbitals in the process. We will not care about this sign as it does not change the energy of the wavefunction.

variation to be very small, so we can write

$$U = e^{i\epsilon M}$$

with $M = M^\dagger$ a Hermitian matrix[23]. With ϵ small, we have

$$U = \mathbf{1} + i\epsilon M + \ldots$$

which we plug into Eq. 7.27 to give

$$\tilde{c}^\dagger_\mu = c^\dagger_\mu + i\epsilon \sum_\nu M_{\mu\nu} c^\dagger_\nu + \ldots$$

Here, as mentioned above, to have any change in the resulting Slater determinant we are only interested in M that mixes filled and empty orbitals. Thus we can assume that $M_{\mu\nu}$ is nonzero only if either μ is filled and ν is empty or ν is filled and μ is empty. (in particular $\mu \neq \nu$).

Thus we consider trial states of the form

$$\begin{aligned} |\Psi\rangle_\epsilon &= \prod_{\mu\,\text{filled}} \tilde{c}^\dagger_\mu |0\rangle \\ &= \prod_{\mu\ \text{filled}} \left(c^\dagger_\mu + i\epsilon \sum_{\nu\ \text{empty}} M_{\mu\nu} c^\dagger_\nu \right) |0\rangle \end{aligned} \tag{7.28}$$

where the sum over ν must be only over unoccupied states, such that we have μ occupied and ν unoccupied (or equivalently M is simply zero for all other cases). We now want to expand this product order by order in ϵ. We get

$$|\Psi\rangle_\epsilon = \left[\prod_{\mu\ \text{filled}} c^\dagger_\mu |0\rangle \right] + i\epsilon \sum_{\nu\ \text{empty};\ \mu\ \text{filled}} M_{\mu\nu} c^\dagger_\nu c_\mu \left[\prod_{\lambda\ \text{filled}} c^\dagger_\lambda |0\rangle \right] + \ldots$$

Let us walk through this result in some more detail. The first term in brackets, the product of the $c^\dagger_\mu$ is the product of all of the first terms in Eq. 7.28. This just gives the unperturbed ground state $|\text{GS}\rangle$ (ie., the $\epsilon = 0$ wavefunction). The order ϵ^1 term is more complicated. To get this term from the product of Eq. 7.28 one chooses only a single μ in the product where instead of taking the first term $c^\dagger_\mu$ one instead chooses the $M_{\mu\nu}$ term[24]. We write this term in a creative way, by starting with $|\text{GS}\rangle$ (the term in square brackets on the far right) and removing the orbital μ with c_μ and then putting in the sum over $M_{\mu\nu} c^\dagger_\nu$ instead. As a shorthand we can write

$$|\Psi\rangle_\epsilon = |\text{GS}\rangle + \epsilon |\delta\Psi\rangle + \ldots$$

---

[23] Let us check that exponentiating a hermitian matrix gives a unitary matrix. For a matrix to be unitary we must have $UU^\dagger = \mathbf{1}$. So let us check $(e^{i\epsilon M})(e^{i\epsilon M})^\dagger = (e^{i\epsilon M})(e^{-i\epsilon M}) = \mathbf{1}$.

[24] If a sign occurs in reordering creation operators this can be absorbed into M.

where

$$|\delta\Psi\rangle = i\epsilon \sum_{\nu \text{ empty; } \mu \text{ filled}} M_{\mu\nu} c^\dagger_\nu c_\mu \, |\mathrm{GS}\rangle \tag{7.29}$$

At this linear order in ϵ it is easy to see that

$$\langle \delta\Psi | \mathrm{G}S\rangle = 0$$

since $\delta\Psi$ always has some orbitals ν filled which are not filled in the ground state, GS. This then implies that

$${}_\epsilon\langle \Psi | \Psi \rangle_\epsilon = 1 + \mathcal{O}(\epsilon^2)$$

Finally we turn to the variational condition. We would like our wavefunction to be at an extremum of the energy. Thus we want

$$\left.\frac{\partial E}{\partial \epsilon}\right|_{\epsilon=0} = 0$$

which we write as

$$\left.\frac{\partial}{\partial \epsilon}\right|_{\epsilon=0} \frac{{}_\epsilon\langle \Psi | H | \Psi \rangle_\epsilon}{{}_\epsilon\langle \Psi | \Psi \rangle_\epsilon} = 0$$

where this condition should now be true for *any* hermitian matrix M that mixes filled and unfilled orbitals. Note that the denominator of this fraction we just found to be 1 up to corrections of order ϵ^2 so we can throw this out. Expanding our condition and taking the ϵ derivative gives us the condition

$$0 = \langle \delta\Psi | H | \mathrm{GS}\rangle + \langle \mathrm{GS} | H | \delta\Psi\rangle = \mathrm{Re}\langle \mathrm{GS} | H | \delta\Psi\rangle$$

And indeed since this needs to be true for any matrix M in Eq. 7.29, we can equivalently state the condition

$$\mathrm{Re}\langle \mathrm{GS} | H c^\dagger_\nu c_\mu | \mathrm{GS}\rangle = 0$$

where μ is filled in the ground state GS and ν is empty in the ground state GS. Writing H out explicitly we get

$$\mathrm{Re}\langle \mathrm{GS}| \left[\sum_{\alpha\beta} h_{\alpha\beta} c^\dagger_\alpha c_\beta + \sum_{\alpha\beta\gamma\delta} \frac{1}{2} v_{\alpha\beta\gamma\delta} c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \right] c^\dagger_\nu c_\mu \, |\mathrm{GS}\rangle = 0 \tag{7.30}$$

Let us attack this term by term. In the first term, we have

$$\langle \mathrm{GS} | c^\dagger_\alpha c_\beta c^\dagger_\nu c_\mu \, |\mathrm{GS}\rangle$$

Since μ is occupied (filled) and ν is unoccupied (empty) in $|GS\rangle$, this expression can only be nonzero if $\mu = \alpha$ and $\nu = \beta$.

$$\langle \mathrm{GS} | \contraction{}{c^\dagger_\alpha}{\, c_\beta \, c^\dagger_\nu \,}{c_\mu} \contraction[2ex]{c^\dagger_\alpha \,}{c_\beta}{\,}{c^\dagger_\nu} c^\dagger_\alpha \, c_\beta \, c^\dagger_\nu \, c_\mu \; |\mathrm{GS}\rangle = \delta_{\nu\beta}\delta_{\alpha\mu}$$

Thus the first term in the correlator Eq.7.30 is simply $h_{\mu\nu}$.

We next examine the second, more complicated, term in Eq. 7.30. This has the form

$$\langle \mathrm{GS}|\; c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \; c^\dagger_\nu c_\mu \;|\mathrm{GS}\rangle$$

Now there are four different ways in which this can be nonzero, which we now list here. For all of these we must have μ initially filled and ν initially empty.

$$\begin{array}{lcll}
\wick{\langle \mathrm{GS}|\; \c1 c^\dagger_\alpha \c2 c^\dagger_\beta \c2 c_\delta \c3 c_\gamma \; \c3 c^\dagger_\nu \c1 c_\mu \;|\mathrm{GS}\rangle} & \to & +\delta_{\alpha\mu}\delta_{\beta\delta}\delta_{\gamma\nu} & \delta \text{ initially filled} \\
\wick{\langle \mathrm{GS}|\; \c1 c^\dagger_\alpha \c2 c^\dagger_\beta \c3 c_\delta \c1 c_\gamma \; \c3 c^\dagger_\nu \c2 c_\mu \;|\mathrm{GS}\rangle} & \to & +\delta_{\alpha\gamma}\delta_{\beta\mu}\delta_{\delta\nu} & \gamma \text{ initially filled} \\
\wick{\langle \mathrm{GS}|\; \c1 c^\dagger_\alpha \c2 c^\dagger_\beta \c3 c_\delta \c2 c_\gamma \; \c3 c^\dagger_\nu \c1 c_\mu \;|\mathrm{GS}\rangle} & \to & -\delta_{\alpha\mu}\delta_{\beta\gamma}\delta_{\delta\nu} & \gamma \text{ initially filled} \\
\wick{\langle \mathrm{GS}|\; \c1 c^\dagger_\alpha \c2 c^\dagger_\beta \c1 c_\delta \c3 c_\gamma \; \c3 c^\dagger_\nu \c2 c_\mu \;|\mathrm{GS}\rangle} & \to & -\delta_{\alpha\delta}\delta_{\beta\mu}\delta_{\gamma\nu} & \delta \text{ initially filled}
\end{array}$$

Putting these results together we obtain the condition

$$h_{\mu\nu} + \frac{1}{2} \sum_{x \text{ occupied}} \left[v_{\mu x \nu x} + v_{x \mu x \nu} - v_{\mu x x \nu} - v_{x \mu x \nu} \right] = 0$$

Now using the symmetry of v given in Eq. 7.13 we find that the first two v terms are the same and the last two v terms are the same thus giving us

$$h_{\mu\nu} + \sum_{x \text{ occupied}} \left[v_{\mu x \nu x} - v_{\mu x x \nu} \right] = 0$$

for all μ filled and ν empty. We recognize the sum over x as being precisely $f_{\mu\nu}$ as given in Eq. 7.25. So our condition is

$$h_{\mu\nu} + f_{\mu\nu} = 0$$

for μ initially filled and ν initially unfilled. Thus if we started with a Hartree-Fock basis, where $h+f$ is diagonal, this condition in necessarily satisfied (since it will only be nonzero for $\mu = \nu$). Thus we conclude that the solution to the Hartree-Fock equations indeed produces a single Slater determinant with its energy extremized! QED. $\square$. Yay. etc.

7.5 Application of Hartree-Fock to Translationally Invariant Fermions

We now would like to apply Hartree-Fock theory to a very simple, but also very important case — the translationally invariant interacting Fermi gas.

This situation is supposed to model electrons in metals, but we have thrown away the crystal lattice for simplicity and just kept the electrons. (So, for example, we will have a perfectly spherical Fermi sea, as compared to what we get in real metals). Note that if we completely throw away the positive ions in the crystal lattice, the Coulomb energy of all the electrons interacting with each other becomes infinite. To avoid this problem, one usually smears out a neutralizing positive charge which we keep along with the electrons, so that the entire system is charge neutral (but still completely translationally invariant). This model is known as the "jellium" model[25] (with the idea that the positive charge is like a smeared out jelly that has been spread evenly around the system).

Another way to handle the problem coming from the infinite Coulomb interaction is to just consider fermions with shorter range interaction $V(\mathbf{r})$. While this does not apply to real electrons, it does apply to Fermi systems such as ^{3}He.

Whether we use a jellium background or not, our Hamiltonian will always be of the form

$$H = H_0 + H_{int}$$

where

$$H_0 = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 \mathbf{k}^2}{2m} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

is the kinetic (single particle, noninteracting part) of the Hamiltonian, and

$$H_{int} = \frac{1}{2} \sum_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} \;\; c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{\mathbf{k_2}\sigma_2} c_{\mathbf{k_4}\sigma_4} c_{\mathbf{k_3}\sigma_3}$$

Note when comparing to the form written in Eq. 7.11 the indices we used as a, b, c, d are now replaced by the combined indices $(\mathbf{k}_1\sigma_1), (\mathbf{k}_2\sigma_2), (\mathbf{k}_3\sigma_3), (\mathbf{k}_4\sigma_4)$. The matrix element is given by

$$v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} = \langle \mathbf{k}_1\sigma_1; \mathbf{k}_2\sigma_2 | V(\mathbf{r}-\mathbf{r}') | \mathbf{k}_3\sigma_3; \mathbf{k}_4\sigma_4 \rangle$$

Here the kets are normalized (but unsymmetrized) plane wave state of two particles

$$\langle \mathbf{r}\sigma_3; \mathbf{r}'\sigma_4 | \mathbf{k}_3\sigma_3; \mathbf{k}_4\sigma_4 \rangle = \frac{1}{\mathcal{V}} \; e^{i\mathbf{k}_3\cdot\mathbf{r} + i\mathbf{k}_4\cdot\mathbf{r}'}$$

with $\mathcal{V}$ the volume of the system. Thus we have

$$\begin{aligned} v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} &= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} \int d\mathbf{r} \int d\mathbf{r}' \frac{1}{\mathcal{V}^2} e^{-i\mathbf{k}_1\cdot\mathbf{r} - i\mathbf{k}_2\cdot\mathbf{r}'} e^{i\mathbf{k}_3\cdot\mathbf{r} + i\mathbf{k}_4\cdot\mathbf{r}'} V(\mathbf{r}-\mathbf{r}') \\ &= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} \frac{1}{\mathcal{V}} \delta_{\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3+\mathbf{k}_4} \tilde{V}(\mathbf{k}_4 - \mathbf{k}_2) \end{aligned}$$

---

[25] The Jellium model (including the name) was constructed by Conyers Herring. Herring was an extremely important condensed matter physicist in the mid 1900s — and his influence was often in the background of other great works. Herring was the first head of the famous Bell Labs theory department. Many years later, when Bell Labs was closing down its fundamental research effort, I was the last head of the Bell Labs theory department – a rather dubious distinction I'm afraid.

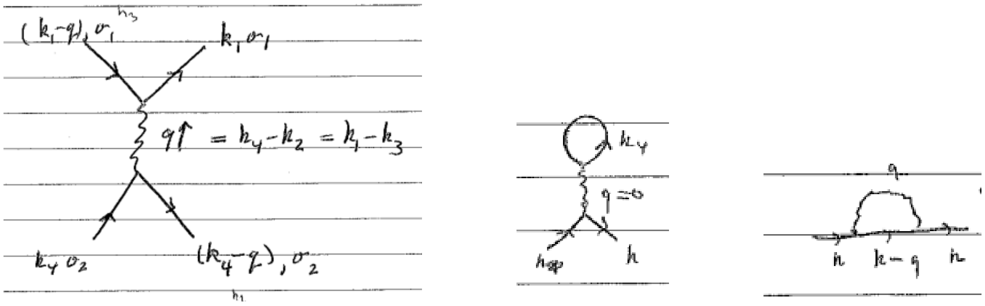

Figure 7.2: Left: The interaction in Eq. 7.31 drawn as a diagram. Middle: connecting up the legs of the diagram to make the Hartree contribution. Right: Connecting the legs up to make the Fock contribution.

where

$$\tilde{V}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} V(\mathbf{r})$$

We can thus rewrite

$$H_{int} = \frac{1}{2\mathcal{V}} \sum_{(\mathbf{k_1},\sigma_1),(\mathbf{k}_4,\sigma_4),\mathbf{q}} c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \tilde{V}(\mathbf{q}) \tag{7.31}$$

Note that there is another, potentially more physical way to write this expression

$$H_{int} = \sum_{\mathbf{q}} : \rho(\mathbf{q}) \tilde{V}(\mathbf{q}) \rho(-\mathbf{q}) :$$

where ρ is the density written in Fourier space

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{k}\sigma} = \mathrm{FourierTransform}_{\mathbf{q}}[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})] \tag{7.32}$$

Although we don't intend to express our perturbation theory in terms of Feynman diagrams, it is occassionally useful to write these diagrams anyway — not the least reason being that one will often see these diagrams in the literature, and it is useful to be able to convert the diagram into physical expressions. The interaction 7.31 can be written diagrammatically as shown in the left of Fig. 7.2. When we make the Hartree-Fock approximation, we want to average one creation and one annihilation operator to give $\langle c^\dagger_a c_b \rangle$, and this can be done in two ways, corresponding to the direct and exchange (Hartree and Fock) terms.

The first possibility is the direct or Hartree term

$$\overbrace{c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}}$$

and the second is the exchange or Fock term

$$c^\dagger_{\mathbf{k_1}\sigma_1}\overbrace{c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4}c_{\mathbf{k_4}\sigma_4}c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}}$$

We will examine these one at a time.

Note that we are going to assume that the ground state is in the form of a Fermi sea

$$|\mathrm{FS}\rangle = \prod_{\sigma,\mathbf{k}<k_F} c^\dagger_{\mathbf{k}\sigma}|0\rangle$$

and we will justify this assumption post-facto.

Direct (Hartree) Term

We have

$$H_{Hartree} = \frac{1}{\mathcal{V}}\sum_{\mathbf{q}}\left[\sum_{\mathbf{k_1},\sigma_1}\langle c^\dagger_{\mathbf{k_1}\sigma_1}c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle\right]\sum_{\mathbf{k_4},\sigma_4}c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4}c_{\mathbf{k_4}\sigma_4}\tilde{V}(\mathbf{q})$$

Here we examine the expectation. If we are taking the expection in a Fermi sea state, we have

$$\langle c^\dagger_{\mathbf{k_1}\sigma_1}c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle = \delta_{\mathbf{q},0}\times n_F(\mathbf{k})$$

where

$$n_F(\mathbf{k}) = \begin{cases} 1 & |\mathbf{k}|<k_F \\ 0 & \text{otherwise}\end{cases} \tag{7.33}$$

is the Fermi occupation factor at zero temperature for the Fermi sea where k_F is the Fermi wavevector. Thus the expression in the square brackets is

$$\left[\sum_{\mathbf{k_1},\sigma_1}\langle c^\dagger_{\mathbf{k_1}\sigma_1}c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle\right] = N\delta_{\mathbf{q},0}$$

with N the total particle number. We then get

$$H_{Hartree} = \frac{N}{\mathcal{V}}\tilde{V}(0)\sum_{\mathbf{k}_4,\sigma_4}c^\dagger_{\mathbf{k_4}\sigma_4}c_{\mathbf{k_4}\sigma_4}$$

This is nothing more than a shift of the chemical potential and is therefore trivial. Indeed, if one considers a jellium model where the positive charge is neutralized by a uniform background charge, $\tilde{V}(0)=0$, and this term vanishes exactly. Diagramatically, this is expressed by the diagram in the middle of Fig. 7.2.

Exchange (Fock) Term

Here we have

$$H_{Fock} = \frac{-1}{\mathcal{V}} \sum_{\mathbf{k_1},\sigma_1} \left[\sum_{\mathbf{k}_4,\sigma_4,\mathbf{q}} \langle c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \rangle \tilde{V}(\mathbf{q}) \right] c^\dagger_{\mathbf{k_1}\sigma_1} c_{\mathbf{k_4}\sigma_4}$$

We again examine the expectation in the Fermi sea ground state giving us

$$\langle c^\dagger_{((\mathbf{k_4}-\mathbf{q})\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \rangle = \delta_{\sigma_1,\sigma_4} \delta_{k_1,k_4} \; n_F(\mathbf{k}_4 - \mathbf{q})$$

so the Fermi occupation factor here is unity only if $|\mathbf{k}_4 - \mathbf{q}| < k_F$ and is otherwise zero. We can then write the Fock term as

$$H_{Fock} = \sum_{\mathbf{k},\sigma} \Sigma_{Fock}(\mathbf{k}) \; c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where Σ_{Fock} is known as the *self-energy* and is given by

$$\Sigma_{Fock}(\mathbf{k}) = -\frac{1}{\mathcal{V}} \sum_{\mathbf{q}} \tilde{V}(\mathbf{q}) n_F(|\mathbf{k} - \mathbf{q}|)$$

Diagrammatically this result is shown in the far right of Fig. 7.2.

Putting the Hartree-Fock pieces together

Adding together the Hartree and Fock contributions we get the effective Hartree-Fock Hamiltonian

$$H_{HF} = \sum_{\mathbf{k},\sigma} \epsilon_{HF}(\mathbf{k}) \, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma} \tag{7.34}$$

where

$$\epsilon_{HF}(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m} + \frac{N}{\mathcal{V}} \tilde{V}(0) + \Sigma_{Fock}(\mathbf{k}) \tag{7.35}$$

What is crucial to note here is that Eq. 7.34 is “diagonal” in the variables $\mathbf{k}$ and σ. This means we have the correct Hartree-Fock eigenstates. Recall that we were supposed to iterate Hartree-Fock until we converge to diagonal. Here we simply guessed the right starting wavefunction, and we found it was diagonal immediately. This may seem surprising, but actually it is not. Before we turned on the interaction, we had a translationally invariant system with a ground state which was a simple Fermi sea. When the interaction was turned on, we did not ruin translational invariance, and this greatly constrains what kind of wavefunctions we can write down. In particular, each Hartree-Fock eigenstate must be an eigenstate of momentum. As a result, the Hartree-Fock best single Slater determinant is simply the filled non-interacting Fermi sea. And in this case, Hartree-Fock just gives a modification to $\epsilon(\mathbf{k})$. This results is the same as what we would get for first order perturbation theory in this case, although that is not always true for Hartree-Fock in non-translationally invariant systems.

It is worth looking at the three terms in Eq. 7.35. The first term is simply the noninteracting kinetic energy. When we sum this up over the entire Fermi sea in Eq. 7.34 we obtain (this is an easy exercise to show!)

$$E_0 = \frac{3}{5} N E_F^0 \tag{7.36}$$

where E_F^0 is the noninteracting Fermi energy. The total Hartree energy summed over all of the particles is

$$E_{Hartree} = \frac{1}{2}\frac{N^2}{\mathcal{V}}\tilde{V}(0) \tag{7.37}$$

with $\mathcal{V}$ the volume of the system as usual; and the total Fock energy summed over all the particles is

$$E_{Fock} = \frac{-1}{2\mathcal{V}} \sum_{\mathbf{q},\mathbf{q}',\sigma} n_F(\mathbf{q}) n_F(\mathbf{q}') \tilde{V}(\mathbf{q}-\mathbf{q}') \tag{7.38}$$

Note that this rather intuitive expresion gives only interaction between aligned spins, as is required for the Fock term. The factors of 1/2 in Eq.7.37 and 7.38 are included to avoid overcounting as described in Eq. 7.26.

7.5.1 Hartree-Fock Effective Mass

The interesting physics of a metal is often the low energy physics compared to E_F, since E_F for a metal is often huge. We are thus interested in the low energy excitations near the Fermi surface.

For a noninteracting Fermi gas we can expand around the Fermi surface and write

$$\begin{aligned} \epsilon^0(\mathbf{k}) &= E_F + \frac{\hbar k_F}{m}\hbar(|\mathbf{k}| - k_F) \\ &= E_F + v_F\, \hbar(|\mathbf{k}| - k_F) \end{aligned}$$

where we have defined the Fermi velocity to be

$$v_F = \hbar k_F / m$$

Note that we are dropping terms which are $(|\mathbf{k}| - k_F)^2$ and higher powers being that we are assuming we are close to the Fermi surface.

For an interacting Fermi system we can write instead

$$\epsilon(\mathbf{k}) = E_F^* + \frac{\hbar k_F}{m^*}\hbar(|\mathbf{k}| - k_F)$$

where we have defined an effective mass m^* by

$$\frac{\hbar^2}{m^*} = \left.\frac{\partial^2}{\partial k^2}\epsilon_{HF}(k)\right|_{k=k_F}$$

For example, for ^{3}He, the effective mass ranges from 2-6 times the bare mass of the Helium atom, depending on the pressure applied to the system.

Effective Mass for Coulomb Interaction

We now return to the Coulomb interaction, which is slightly troublesome due to its long range nature. We start with

$$V(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|}$$

which we Fourier transform to get[26]

$$\tilde{V}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|} = \frac{e^2}{\epsilon_0|\mathbf{k}|^2} \tag{7.39}$$

Here we note that $\tilde{V}(0)$ (which we need for the Hartree energy) is divergent for the Coulomb interaction. This is a result of having not included the neutralizing positive (jellium) background. If we put this in, it will fully cancel $\tilde{V}(0)$ and we don't have to worry about this divergence.

Let us now calculate the Fock self-energy

$$\begin{aligned} \Sigma_{Fock}(\mathbf{k}) &= -\frac{1}{\mathcal{V}}\sum_{\mathbf{q}} \tilde{V}(\mathbf{q}) n_F(|\mathbf{k}-\mathbf{q}|) \\ &= \frac{e^2}{\epsilon_0}\frac{1}{\mathcal{V}} \sum_{|\mathbf{k}'|<\mathbf{k_F}} \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} = \frac{e^2}{\epsilon_0}\int_0^{|\mathbf{k}'|=\mathbf{k_F}} \frac{d\mathbf{k}'}{(2\pi)^3}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \end{aligned} \tag{7.40}$$

which is sketched in Fig. 7.3. For $\mathbf{k} = 0$ it is easy to calculate that $\Sigma = e^2 k_f/(\epsilon_0 2\pi^2)$. And it is also easy to see that Σ must decay for very large $\mathbf{k}$. However, what is not as obvious is that the self energy has a log-divergent slope at k_F. The calculation that shows this is given just below.

Given the log divergent slope, m^* then goes to zero at the Fermi surface. The reason for the log divergence is the long-ranged Coulomb interaction. Over long distances, other electrons rearrange themselves to cancel the Coulomb potential, and this is not properly accounted for in simple Hartee-Fock. This rearrangement of charges to remove the long range Coulomb interaction is known as *screening* and will be treated in some detail in the next chapter.

---

[26] On dimensional grounds, and by rotational invariance we know that it has to be proportional to $\frac{1}{|\mathbf{k}|^2}$, so let us call the result $\frac{\alpha}{|\mathbf{k}|^2}$. To get the prefactor right it is useful to look at the inverse Fourier transform

$$V(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\alpha}{|\mathbf{k}|^2}$$

Then take the laplacian

$$\nabla^2 V(\mathbf{r}) = \alpha \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} = \alpha\delta(\mathbf{r})$$

and by Gauss' law we can then fix the prefactor $\alpha = e^2/\epsilon_0$.

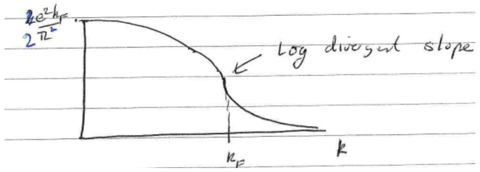

Figure 7.3: A plot of the self-energy in the case of the Coulomb interaction

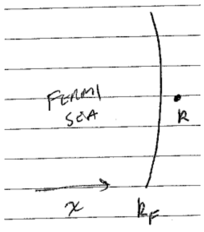

Figure 7.4: A plot of the self-energy in the case of the Coulomb interaction

7.6 Appendix: Showing the Log Divergence at The Fermi Surface

We want to calculate the self energy Eq. 7.40 as $\mathbf{k}$ approaches the Fermi surface. Let us consider $\mathbf{k}$ (without loss of generality) in the x direction and approaching the Fermi surface k_F, as shown in Fig. 7.4. We divide the integral over $\mathbf{k}'$ into an integral in the x direction and an inegral in the directions perpendicular to x, which we call $\mathbf{k}'_\perp$.

$$\begin{aligned}
\Sigma_{HF}(\mathbf{k}) &= \int d\mathbf{k'}_\perp \int dk'_x \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \\
&= \int_{-k_F}^{k_F} dk'_x 2\pi \int_0^{\sqrt{k_F^2-(k'_x)^2}} dk'_\perp k'_\perp \frac{1}{|k-k'_x|^2+k_\perp^2} \\
&\approx 2\pi \int_{-k_F}^{k_F} dk'_x \log(|k-k'_x|^2/\text{cutoff}) \\
&\sim (k-k_F)\log(|k-k_F|)
\end{aligned}$$

Thus we have

$$\frac{\partial \epsilon_{HF}}{\partial k} \sim \log(|k-k_F|)$$

and

$$\frac{1}{m*} \sim \frac{\partial^2 \epsilon_{HF}}{\partial k^2} \sim \frac{1}{|k-k_F|}$$

Chapter 8

Screening and Linear Response

In the previous chapter we had some problems with the long-rangedness of the Coulomb interaction. While we will not completely solve this problem here, we understand that the solution comes from allowing other particles to respond to the potential created, thus *screening* the long range interaction. Indeed, we know that if we try to put a postive charge in a metal at one point and a negative charge at another point (so as to keep the total charge neutral) the other charges in the metal should rearrange so as to make the metal look overall neutral everywhere — at least when looked at from far away.

More generally we are interested in how a system responds to any arbitrary perturbation. We will study this at various levels of sophisitication.

8.1 Thomas-Fermi Screening

Let us consider a uniform electron gas and we imagine there is some potential $U(\mathbf{r})$ that the electrons feel. We thus have a Hamiltonian which is

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i)$$

Let us further assume that $U(\mathbf{r})$ varies slowly in space and $\langle U \rangle = 0$ for simplicity. For example, we might assume that $U(\mathbf{r}) = U_0 \cos(\mathbf{q} \cdot \mathbf{r})$ with small $|\mathbf{q}|$.

To determine what happens in this situation we start by thinking locally: Locally we have a Fermi sea which is filled up to the chemical potential μ. If the potential U increases, this pushes some of the electrons above the chemical potential and the density drops by

$$\delta n(\mathbf{r}) = -D(E_F)U(\mathbf{r}) \tag{8.1}$$

where $D(E_F)$ is the density of states per unit volume. This is shown in Fig. 8.1.

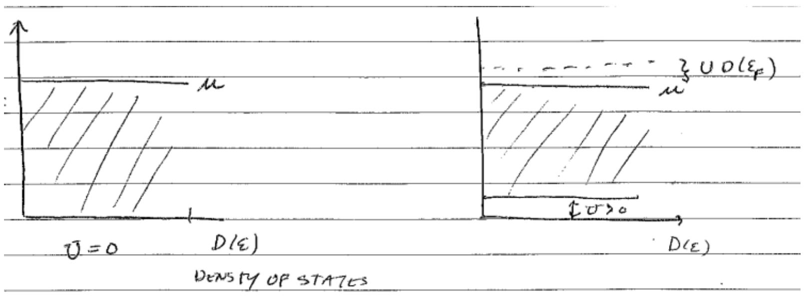

Figure 8.1: Left: States are filled up to the chemical potential μ. Right: If an additional potential U is added to the system, some states are pushed above the chemical potential, and the local density drops by $D(E_F)U$ where D is the density of states per unit volume.

In this situation, we sometimes call the quantity $-D(E_F)$ in Eq. 8.1 a *response function*[1].

At this point, we are still ignoring interactions between the electrons, we are only keeping the interaction between the electrons and the potential U. With more careful thought, we realize that the interaction beween electrons should matter. When the electrons move around in response to the potential U, they then create a new electrostatic potential that the other electrons then should respond to. Thus we need to consider some sort of self-consistent approach. First, however, we should convert our response equation into an equation that explains how charge moves around, rather than how density moves around.[2]

$$\delta\rho(\mathbf{r}) = -e\,\delta n(\mathbf{r})$$

The potential felt by an electron moving in an *electrostatic* potential $\phi(\mathbf{r})$ is

$$U(\mathbf{r}) = -e\phi(\mathbf{r})$$

Thus, our above response equation Eq. 8.1 can be rewritten as a charge response to an electrostatic potential

$$\delta\rho(\mathbf{r}) = -e^2 D(E_F)\phi(\mathbf{r}) \tag{8.2}$$

Now if there is a change in density, there is a resulting change in the electrostatic potential. The resulting electrostatic potential is given by Gauss' law

$$\begin{aligned} \nabla^2\phi &= \frac{-\delta\rho}{\epsilon_0} \\ &= \frac{e^2}{\epsilon_0} D(E_F)\phi \end{aligned} \tag{8.3}$$

---

[1] Later we will call this quantity the response function χ^0 (up to some factors of e). The superscript 0 indicating that it does not yet include interaction between electrons, but only interaction of electrons with the potential U.

[2] This is going to be one of those times when we really wish we could go back in time and tell Benjamin Franklin to switch the definition of positive charge so that the electron is positive! The minus signs here are a common source of error!

where we have used Eq. 8.2 in going to the second line. This resulting equation for ϕ is precisely the self-consistent Hartree equation: Electrons respond to a density which is created by all the other electrons.

It is useful now to define the so-called Thomas-Fermi[3] wavevector[4]

$$k_{TF}^2 = \frac{e^2}{\epsilon_0} D(E_F) \tag{8.4}$$

So that our self consistent screening equation 8.3 is just

$$\nabla^2 \phi = k_{TF}^2 \phi$$

Such an equation has a characteristic decay of the form

$$\phi \sim e^{-k_{TF}|\mathbf{r}|}$$

The potential decays exponentially because it is *screened* by other electrons. To be more precise, let us consider the field near a point charge of strength Q inserted into our system of electrons. The resulting electrostatic potential is given by the Yukawa[5] form

$$\phi = \frac{Q}{4\pi\epsilon_0 |\mathbf{r}|} e^{-k_{TF}|\mathbf{r}|} \tag{8.5}$$

This potential solves the equation

$$\nabla^2 \phi = k_{TF}^2 \phi + \frac{Q}{\epsilon_0} \delta(\mathbf{r})$$

where the second term on the right represents the source charge that is inserted.

Let us now estimate the Thomas-Fermi wavevector. The density of states in a noninteracting Fermi liquid is given by[6]

$$D(E_F) = \frac{3}{2}\frac{n}{E_F} = \frac{m k_F}{\hbar^2 \pi^2}$$

---

[3] Llewelyn Thomas invented this in 1927, frighteningly soon after Fermi-Dirac statistics was invented (1925).

[4] It is worth checking that k_{TF} does indeed have the dimensions of a wavevector. First, note that $D(E_F)$ is is a density of states per unit volume, so it has dimension 1/(Energy – Volume). Next note that $e^2/(\epsilon_0 \times \text{length})$ is an energy. The rest is easy.

[5] Yukawa won a Nobel prize in 1949 for his work on nuclear forces.

[6] To derive this $E \sim k_F^2 \sim n^{2/3}$, so $dE/dn = (2/3)E/n$, and $dn/dE = (2/3)E/n$. We also need $E_F = \hbar^2 k_F^2/(2m)$ and an expression for the density in terms of k_F which is given by

$$n = 2\frac{1}{(2\pi)^3}\frac{4}{3}\pi k_F^3$$

where the prefactor of 2 is for two spin states, the 2π factors are the usual factor that comes with k space integration, and the remaining factor is volume of sphere with radius k_F.

We thus have

$$k_F = \sqrt{\frac{D(E_F)e^2}{\epsilon_0}} = \sqrt{\frac{mk_Fe^2}{\hbar^2\pi^2\epsilon_0}} = \sqrt{\frac{4}{\pi}}\sqrt{\frac{k_F}{a_0}}$$

where a_0 is the Bohr radius. Now in a typical metal we have a screening length $1/k_F \approx a_0 \approx 1$ Angstrom which is very short. However, in a semiconductor, this screening length can be 10-100 Angstroms or more due to a small k_F and a large a_0 (the small k_F coming from a low density of electrons, and the large a_0 coming from a low mass and a large effective dielectric constant).

The Thomas-Fermi approximtion is a good first approach for understanding screening. In particular it removes the long range singularity of the Coulomb interactions. However, there are some things that are obviously wrong with the Thomas-Fermi approach. The main problem is that it is an "instantaneous" approximation, whereas if we add a charge to a system it actually takes some time for the electrons to rearrange so as to screen the charge. This time delay can turn out to be very important. This brings us to the topic of dynamical screening and dynamical response.

8.2 Response More Generally

We will now consider response functions more generally — including time dependent response. Let us generally write our Hamiltonian

$$H = \hat{H}_0 + \delta\hat{H}(t)$$

where $\delta\hat{H}(t)$ is the small perturbation applied to the system (and $\hat{H}_0$ is the Hamiltoninan in the absence of the perturbation). Although we will here be interested in the response of an interacting Fermi liquid to a perturbation, the same principles we use here are far more general and can be applied to many other systems. It is always conventient to assume that the perturbation goes to zero at time $t = -\infty$ and turns on slowly.

An important example of such a perturbation (for our electron system) would be a weak time dependent externally applied electrostatic potential, in which case we have

$$\delta\hat{H}(t) = \int d\mathbf{r}\,(-e\phi_{ext}(\mathbf{r},t)\hat{n}(\mathbf{r})) \tag{8.6}$$

However, we could perturb the system with many other things, such as a magnetic field, or pressure, etc, and much of the calculation of response will be similar.

We now want to ask how the system responds to this perturbation. To probe this response we measure some observable operator $\hat{B}$. So we are interested in

$$\langle\hat{B}\rangle_t = \langle\psi(t)|\hat{B}|\psi(t)\rangle$$

where $|\psi(t)\rangle$ is the time dependent many-particle wavefunction.

An example here is that we might be interested in the density operator

$$\hat{B} = \delta n(\mathbf{r}).$$

So, for example, if we perturb (in Eq. 8.6) with the potential $\phi(\mathbf{r}, t)$ we might ask what is the resulting change in density at some later time.

One key priniciple to keep in mind is that of causality: If a perturbation occurs at time t we should only have a response at times $t' \geqslant t$.

Time Dependent Perturbation Theory

So how are we going to find the general response $\langle \hat{B} \rangle_t$? The strategy here is to assume the perturbation $\delta\hat{H}(t)$ is small and use time dependent perturbation theory.

Let us start with the time dependent Schroedinger equation.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_S = \left[H_0 + \delta\hat{H}(t) \right] |\psi(t)\rangle_S$$

The subscript S here indicates that the kets are in the Schroedinger representation. Also note that inside the square brackets is the full Hamiltonian — which is a combination of the bare part H_0 and the small perturbation.

We now switch to so-called "interaction" representation.

$$|\psi(t)\rangle_I = e^{iH_0 t/\hbar} |\psi(t)\rangle_S$$

In this representation, operators have an additiona time dependence

$$\begin{array}{lll} \hat{B} & \rightarrow \hat{B}_I(t) & = e^{iH_0 t/\hbar} \; \hat{B}_S \; e^{-iH_0 t/\hbar} \\ \delta\hat{H} & \rightarrow \delta\hat{H}_I(t) & = e^{iH_0 t/\hbar} \; \delta\hat{H}_S \; e^{-iH_0 t/\hbar} \end{array}$$

In this representation, the Schroedinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = \delta\hat{H}(t) \; |\psi(t)\rangle_I \tag{8.7}$$

Note that in this representation, if $\delta H = 0$ then $|\psi\rangle_I$ is actually time independent.

We can now write out a formal solution of the Schroedinger equation in the form

$$|\psi(t)\rangle_I = |\psi\rangle_{I0} - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \delta\hat{H}_I(t') |\psi\rangle_{I0} + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \delta\hat{H}_I(t') \delta\hat{H}_I(t'') |\psi\rangle_{I0} + \ldots \tag{8.8}$$

where $|\psi\rangle_{I0}$ is the wavefunction in the absence of the perturbation, in the interaction rep (and it is therefore a time independent ket). We can confirm that Eq. 8.8 solves the Schroedinger equation Eq. 8.7 by plugging the expansion into both sides of the Schroedinger equation.

We will now make use of the fact that $\delta\hat{H}$ is small and we will truncate the expansion at first order, throwing away terms of order $(\delta\hat{H})^2$ and higher. We can then use the time dependent wavefunction in Eq. 8.8 to calculate the time dependence of some operator to be observed

$$\begin{aligned}
&\langle\hat{B}\rangle_t = \langle\psi_I(t)|\hat{B}_I(t)|\psi_I(t)\rangle \\
&= \left[{}_{I0}\langle\psi| + \frac{i}{\hbar}\int_{-\infty}^{t} dt' \;{}_{I0}\langle\psi|\delta\hat{H}_I(t')\right]\hat{B}_I(t)\left[|\psi\rangle_{I0} - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\delta\hat{H}_I(t')|\psi\rangle_{I0}\right] \\
&= {}_{I0}\langle\psi_I|\hat{B}_I(t)|\psi_I\rangle_{I0} - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \;\;{}_{I0}\langle\psi|\,[\hat{B}_I(t),\delta\hat{H}_I(t')]|\psi\rangle_{I0}
\end{aligned}$$

The first term in the last line is just the value of $\langle B\rangle_t$ in the absence of the perturbation. Thus we have a change in the value of B given by

$$\langle\delta\hat{B}\rangle_t = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \;\; \langle[\hat{B}_I(t),\delta\hat{H}_I(t')]\rangle$$

where the expectation is taken in the unperturbed state $|\psi\rangle_{I0}$ as above. This formula is a general linear response equation, otherwise known as the Kubo formula[7]. The importance of this type of formula can hardly be overstated, as it is used universally to calculate the response of a system to a perturbation.

It is crucial to note that the response here is *linear* in the perturbation (hence the name "linear response"). Linearity gives us the important principle that response of a sum of perturbations is the sum of the responses of each individual perturbation. This will allow us to decompose a general perturbation into a convenient basis of elementary simple perturbations, which will simplify the calculation greatly.

Example of Externally Applied Potential

Let us go back to the main example we want to study: the density response to an externally applied potential. The perturbation is generally of the form

$$\delta\hat{H}_S(t') = \int d\mathbf{r}\left(-e\phi_{ext}(\mathbf{r},t')\hat{n}_S(\mathbf{r})\right) \tag{8.9}$$

with the operators being expressed here in the Schroedinger representation. The operator we would like to measure is again the density operator

$$\hat{B} = \hat{n}_S(\mathbf{r}) \tag{8.10}$$

It is often easier to work in Fourier space. By using Parseval's theorem[8] we have

$$\delta\hat{H}_S(t) = \frac{-e}{\mathcal{V}}\sum_{\mathbf{k}}\phi_{ext}(\mathbf{k},t')\,\hat{n}_S(-\mathbf{k}) \tag{8.11}$$

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[7] Named for the Japanese physicist Ryogo Kubo who constructed this general formula in 1957.

[8] Named for Marc-Antoine Parseval des Chênes who published it in 1799 without proof, stating that it was self-evident.

with $\mathcal{V}$ the volume as usual. Since we are considering *linear* response, we can imagine applying a single wavevector perturbation $\mathbf{k}$ — and if we have an initial perturubation which is a sum of different wavevectors we can just add up the responses to each wavevector at the end of the calculation.

We also write the quantity we want to measure (the density) in $\mathbf{k}$-space

$$\delta B = \delta \hat{n}_S(\mathbf{k})$$

again in the Schroedinger representation.

We can then write our Kubo formula as

$$\begin{aligned} \langle \delta n(\mathbf{k}) \rangle_t &= \frac{ie}{\hbar \mathcal{V}} \int_{-\infty}^{t} dt' \; \langle [\hat{n}_I(\mathbf{k}, t), \hat{n}_I(-\mathbf{k}, t')] \rangle \phi_{ext}(\mathbf{k}, t') && (8.12) \\ &= \int_{-\infty}^{\infty} dt' \; \tilde{\chi}(\mathbf{k}, t - t') \phi_{ext}(\mathbf{k}, t') && (8.13) \end{aligned}$$

where

$$\tilde{\chi}(\mathbf{k}, t - t') = \theta(t - t') \frac{ie}{\hbar \mathcal{V}} \langle [\hat{n}_I(\mathbf{k}, t), \hat{n}_I(-\mathbf{k}, t')] \rangle$$

and

$$\theta(x) = \left\{ \begin{array}{ll} 1 & x > 0 \\ 0 & x < 0 \end{array} \right.$$

is the usual step function. The insertion of the step function in Eq.8.13 implements the correct boundary conditions given explicitily in Eq. 8.12. The function $\tilde{\chi}$ is known as the *linear response function* (or the *susceptibility* or the *linear response kernel*) and note that it is translationally invariant in time. I.e., if we perturb a system at time 0 and measure at time a, this is the same as perturbing at time b and measuring at time $a + b$.

Note that here on the left hand side of Eq. 8.12, we have indicated the response at wavevector $\mathbf{k}$ which was the same wavevector which we perturbed with on the right. In other words we are assuming that the response is diagonal in wavevector. It turns out that this is necessarily true in any tranlationally invariant system — a system that is perturbed at some wavevector $\mathbf{k}$, in linear response theory, will only only respond at the same wavector. We will prove this statement below.

Our next step is to realize that the integral in Eq. 8.13 is a convolution in the t variables. As is usual with a convolution, it is then conventient to Fourier transform. Further, we remember that since we are thinking about *linear* response, we can always decompose the perturbation into a sum of pieces and think about the response to each piece separately. Thus let us just think about a perturbation at a fixed frequency

$$\phi_{ext}(\mathbf{k}, t) = e^{-i\omega t} \phi_{ext}(\mathbf{k}, \omega)$$

If we have a more complicated time dependence we can always sum over many frequencies.

Note that we had previously decided that to make sure things are well-behaved, we want to make sure the perturbation is turned off at time $t = -\infty$. Thus we write instead

$$e^{-i(\omega + i\varepsilon)t} \tag{8.14}$$

where ε is an infinitesimle positive number. This will then properly vanish at $t = -\infty$. We will often not write the $+i\varepsilon$ but we should remember that it is there.

The integral Eq. 8.13 in Fourier space instead reads

$$\delta n(\mathbf{k}, \omega) = \chi(\mathbf{k}, \omega)\phi_{ext}(\mathbf{k}, \omega)$$

where the response χ is given by

$$\begin{aligned} \chi(\mathbf{k}, \omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, \tilde{\chi}(\mathbf{k}, t) \\ &= \frac{ie}{\hbar \mathcal{V}} \int_{0}^{\infty} dt\, e^{i\omega t} \, \langle [\hat{n}_I(\mathbf{k}, t), \hat{n}_I(-\mathbf{k}, 0)] \rangle \end{aligned} \tag{8.15}$$

Note that the $+i\varepsilon$ we added to ω in Eq. 8.14 regularizes this integral at $t = +\infty$.

Eq. 8.15 has two terms in the commutator. We will consider one of these terms explicitly (and we assume the reader can fill in the rest of the calculation for the second term!). We will assume we are at temperature $T = 0$ and that the system is initially in the ground state, which we write as $|\mathrm{GS}\rangle$. The first term in the commutator is

$$\begin{aligned} \langle \mathrm{GS}|\hat{n}_I(\mathbf{k}, t)\hat{n}_I(-\mathbf{k}, 0)\mathrm{GS}\rangle &= \langle \mathrm{GS}|e^{iH_0 t/\hbar}\hat{n}(\mathbf{k})e^{-iH_0 t/\hbar}\hat{n}(-\mathbf{k})|\mathrm{GS}\rangle \\ &= \sum_m \langle \mathrm{GS}|e^{iH_0 t/\hbar}\hat{n}(\mathbf{k})e^{-iH_0 t/\hbar}|m\rangle \, \langle m|\hat{n}(-\mathbf{k})|\mathrm{GS}\rangle \end{aligned}$$

where we have inserted a complete set of eigenstates $|m\rangle$ in the last line (their corresponding energies will be taken to be E_m with E_{GS} being the ground state energy). Here, and hereafter, we have returned to the Schroedinger representation but for simplicity we no longer put subscripts S on kets and operators.

We now make use of the fact that $\hat{n}(-\mathbf{k}) = \hat{n}^\dagger(\mathbf{k})$ to write

$$\langle \mathrm{GS}|\hat{n}(\mathbf{k}, t)\hat{n}(-\mathbf{k}, 0)\mathrm{GS}\rangle = \sum_m \; e^{i(E_{\mathrm{GS}} - E_m)t} \, \langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle \, \langle m|\hat{n}^\dagger(\mathbf{k})|\mathrm{GS}\rangle$$

At this point we think back to the claim made after Eq. 8.13: That a perturbation at wavevetor $\mathbf{k}$ will only elicit a response at the same wavevector $\mathbf{k}$. We can now see why this is the case. Reading this equation from right to left: We start with the grounds state $|\mathrm{GS}\rangle$ which we assume has momentum zero. The operator $\hat{n}^\dagger(\mathbf{k})$ adds momentum $-\hbar\mathbf{k}$ to the ground state and generates an excited state $|m\rangle$ with momentum $-\hbar\mathbf{k}$. Then the operator $\hat{n}(\mathbf{k})$ removes this momentum and returns us to the ground state. If we had measured a response at a different wavevector $\mathbf{k}' \neq \mathbf{k}$, the operator $\hat{n}(\mathbf{k}')$ would not be able to return us to the ground state and we would end up getting zero, as claimed.

We thus have the result

$$\chi(\mathbf{k}, \omega) = \frac{ie}{\hbar \mathcal{V}} \int_0^\infty e^{i\omega t} \sum_m \left\{ e^{i(E_{\mathrm{GS}} - E_m)t/\hbar} |\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle|^2 - e^{-i(E_{\mathrm{GS}} - E_m)t/\hbar} |\langle \mathrm{GS}|\hat{n}(-\mathbf{k})|m\rangle|^2 \right\}$$

where the second term in the brackets is from the other term of the commutator. Taking the integral now gives

$$\chi(\mathbf{k},\omega) = \frac{-e}{\hbar\mathcal{V}}\sum_m \left\{ \frac{|\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_m - E_{\mathrm{GS}})/\hbar} - \frac{|\langle \mathrm{GS}|\hat{n}(-\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_{\mathrm{GS}} - E_m)/\hbar} \right\} \tag{8.16}$$

We now are left with the problem of calculating the matrix elements such as $\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle$. This depends entriely on what particular Hamiltonian we are working with. So far, what we have written is entirely general, and it is still exact at linear response level.

The linear response calculation we have done can be generalized to give the response of any measured operator to any perturbation at linear order. For example, we can generalize the perturbation of Eq. 8.9 to couple to any operator $\hat{A}$

$$\delta H(t) = \int d\mathbf{r}\phi_{ext}(\mathbf{r},t)\hat{A}(\mathbf{r})$$

where ϕ_{ext} is not necessarily an electrostatic potential, and we can measure the respnonse in any operator $\hat{B}(\mathbf{r})$. If we again Fourier transoform to frequency and wavevector we can very generally write

$$\delta B(\mathbf{k},\omega) = \chi_{BA}(\mathbf{k},\omega)\phi_{ext}(\mathbf{k},\omega)$$

and essentially the same calculation will give the response function

$$\chi_{AB}(\mathbf{k},\omega) = \frac{1}{\hbar\mathcal{V}}\sum_m \left\{ \frac{\langle \mathrm{GS}|\hat{B}(\mathbf{k})|m\rangle\langle m|\hat{A}(-\mathbf{k})|\mathrm{GS}\rangle}{\omega + i\varepsilon - (E_m - E_{\mathrm{GS}})/\hbar} - \frac{\langle \mathrm{GS}|\hat{A}(-\mathbf{k})|m\rangle\langle m|\hat{B}(\mathbf{k})|\mathrm{GS}\rangle}{\omega + i\varepsilon - (E_{\mathrm{GS}} - E_m)/\hbar} \right\}$$

8.3 Lindhard Response Function (Response of Noninteracting Electrons)

Let us return to the density-response function Eq. 8.16. While this is a very general equation it is usually very hard to know what the eigenstates $|m\rangle$ and eigenenergies E_m are for a complicated system. So, let us consider a very system to start with: free electrons. We take

$$H_0 = \sum_i \frac{\mathbf{p}_i^2}{2m}$$

only. (In principle, one might want to include interactions in the Hamiltonian — which we will do later, at least in some approximation. However, writing down a complete set of eigenstates is extremely hard when we have interactions, whereas it is fairly easy for the noninteracting case). In this noninteracting case, the ground state $|\mathrm{GS}\rangle$ is simply the filled Fermi sea. We can write the density operator again as (See Eq. 7.32, with apologies that we changed notation for ρ to $\hat{n}$)

$$\hat{n}(\mathbf{k}) = \sum_{\mathbf{q},\sigma} c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma}c_{\mathbf{q}\sigma} = \mathrm{FourierTransform}_{\mathbf{k}}[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})] \tag{8.17}$$

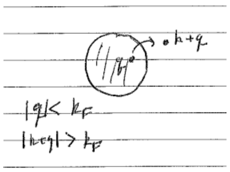

Figure 8.2: The relevant excitations for this calculation are excitations of a single electron out of the Fermi sea.

We thus see that $\hat{n}(\mathbf{k})$ can excite a single electron out of the Fermi sea. Thus, the intermediate states $|m\rangle$ are all of the form

$$|m\rangle = c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{q}\sigma} |\text{GS}\rangle$$

with $|\mathbf{q}| < k_F$ and $|\mathbf{k}+\mathbf{q}| > k_F$ as shown in Fig. 8.2. The corresponding energy difference is given by

$$E_m - E_{\text{GS}} = \frac{\hbar^2 |\mathbf{k}+\mathbf{q}|^2}{2m} - \frac{\hbar^2 |\mathbf{q}|^2}{2m} = \epsilon^0_{\mathbf{k}+\mathbf{q}} - \epsilon^0_{\mathbf{q}}$$

where $\epsilon^0_{\mathbf{q}} = \hbar^2 |\mathbf{q}|^2/(2m)$ as usual, the superscript 0 indicating that this is the energy of noninteracting electrons. Plugging these results into Eq. 8.16, and using $\chi(\mathbf{k}) = \chi(-\mathbf{k})$ we obtain (See chapter appendix for the relevant algebra!)

$$\chi^0(\mathbf{k},\omega) = \frac{-e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\mathbf{q}) - n_F(\mathbf{q}+\mathbf{k})}{\hbar(\omega + i\varepsilon) - (\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})} \tag{8.18}$$

with n_F the Fermi function, which is simply a step function at the Fermi surface at zero temperature (See Eq. 7.33). The superscript 0 here on χ^0 indicates that we are thinking about noninteracting electrons. This rather important result is known as the Lindhard response function[9].

Aside: Green's function language

For those who like to think in Feynman diagrams and Green's functions it is sometimes useful to rephrase our result in this language. For those who are not familiar with this technique, it is OK to mostly ignore it (it is not examinable in this course) and skip down to section 8.3.1. It is simply useful to be able to speak different languages sometimes.

First, the "source" for the response function is the density $\hat{n}(\mathbf{k})$, which we think of in the form of Eq. 8.17 which therefore includes terms of the form $c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{q}\sigma}$. We write this diagrammatically as the vertex shown in the left of Fig.8.3 We then also write the

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[9] Named for Jens Lindhard who wrote it down for the first time in 1954 — rather late for such an important result to be first discovered, although perhaps this is not surprising being that the Kubo formula had not yet been discovered at this time.

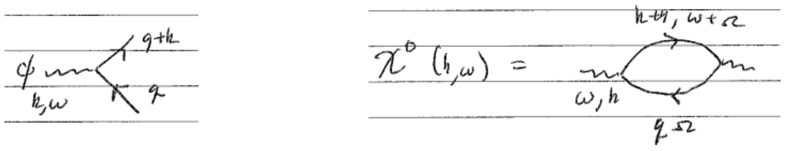

Figure 8.3: Left: Vertex representing a density operator.

Greens' function for the electron as

$$G(\mathbf{k},\Omega) = \frac{1}{\Omega - (\epsilon^0_{\mathbf{k}} - \mu) + i\varepsilon \mathrm{sgn}(\epsilon^0_{\mathbf{k}} - \mu)}$$

which we write as a line with an arrow. The response function χ^0 is then given by the diagram in the right of Fig. 8.3. This diagram corresponds to the integral over the Green's functions

$$\chi^0(\mathbf{k},\omega) = \sum_{\mathbf{q}} \int d\Omega \; G(\mathbf{q},\Omega) G(\mathbf{k}+\mathbf{q},\omega+\Omega)$$

Carrying out the integrals here will generate precisely the same result as Eq 8.18 (up to a prefactor which I may have dropped).

For complicated diagrams, meaning high order perturbation theory calculations, these Green's functions and diagrammatics are a very useful bookkeeping tool. However, at this level it is easier to just do the calculation directly without bothering with diagrams. Nonetheless, it is useful to draw the diagram, because one often sees it in the literature, and it is good to know what it means!

8.3.1 Interpretations

We now would like to interpret the result we have derived Eq. 8.18. We will look at some properties of χ^0, partially to understand it, and partially as a sanity check that we have gotten a reasonable answer!

Imaginary Dissipative Part

First, let us examine the imaginary part of χ. What does it mean that our response function has an imaginary part rather than all real? This simply means that the response is dissipative – energy is absorbed by they system (this is precisely analogous to a conductivity being real rather than imaginary).

To find out when χ^0 has an imaginary part recall that

$$\lim_{\varepsilon \to 0^+} \frac{1}{x + i\varepsilon} = -i\pi\delta(x)$$

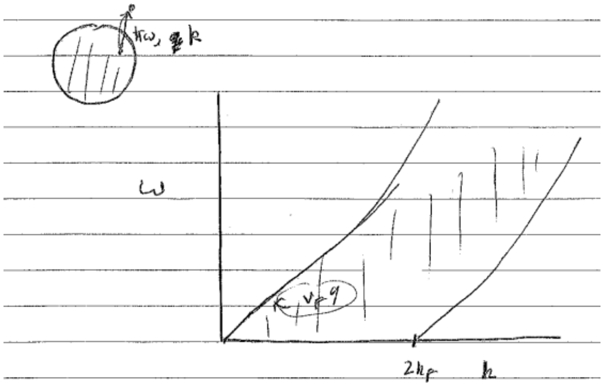

Figure 8.4: The region of q,ω space where there is an imaginary part of χ. This is precisely the region where Eq. 8.19 can be satisfied.

In Eq. 8.18, it is implied that we are taking a limit of $\varepsilon \to 0^+$. Thus the response has an imaginary part when

$$\hbar\omega = \epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}} \quad \text{where} \quad \left\{ \begin{array}{ccc} |\mathbf{q}+\mathbf{k}| > k_F & \text{and} & |\mathbf{q}| < k_F \\ & \text{OR} & \\ |\mathbf{q}+\mathbf{k}| < k_F & \text{and} & |\mathbf{q}| > k_F \end{array} \right. \tag{8.19}$$

In Fig. 8.4 we sketch the region of k, ω space where this condition is satisfied. This is the region of k, ω space where we can add a wavevector $\mathbf{k}$ to the system and get an excitation of energy ω.

Let us make a few quick calculations to determine the rough shape of this region. First we notice that that the longest vector across the Fermi surface is the diameter which is $k = 2k_F$. It is impossible to make any zero energy excitations (ie., from the Fermi surface to the Fermi surface) for wavevectors larger than this. This is why the shaded region in Fig. 8.4 has a boundary at $\omega = 0$ and $k = 2k_F$. Secondly it is useful to look at what happens for small k. Here we can have the condition

$$\hbar\omega = \epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}} = \frac{\hbar^2|\mathbf{k}+\mathbf{q}|^2}{2m} - \frac{\hbar^2|\mathbf{q}|^2}{2m}$$

but for small k we need to have $q \approx k_F$ to satisfy the conditions in Eq. 8.19. Thus we can write

$$\hbar\omega \approx \frac{\hbar k_F}{m} k \cos\theta$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{q}$. The largest ω is then given by $\cos\theta = 1$ or

$$\omega = v_F k$$

with $v_F = \hbar k_F / m$ the Fermi velocity, which is shown in Fig. 8.4.

Low Frequency, Small k

Let us look at the limit $\omega \to 0$ with small k. We then have

$$\chi^0(k,\omega) = \frac{e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\epsilon^0_{\mathbf{q}}) - n_F(\epsilon^0_{\mathbf{q}+\mathbf{k}})}{(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})}$$

where n_F is now a step function in energy at the chemical potential μ. If k is small, then the difference in the denominator is small, as is the difference of the arguments of n_F in the numerator, and we can view the fraction on the right as being a derivative. Since the derivative of a step function is a delta function, we then have

$$\begin{aligned} \chi^0(k,\omega) &= \frac{e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \delta(\epsilon_{\mathbf{q}} - \mu) \\ &= e \int d\epsilon \, D(\epsilon)\delta(\epsilon - \mu) = eD(\mu) \end{aligned}$$

where in going to the second line, we have replaced a sum over $\mathbf{q}$ as an integral over energy times a density of states $D(\epsilon)$. The final result here is just the density of states, which is the static compressibility we derived previously (See Eq. 8.2).

8.3.2 High Frequency $\omega \gg E_F$ and small k

Another limit we can consider is that of high frequency.

Explicit Limit

Here we expand the denominator of Eq. 8.18 for large ω obtaining

$$\chi^0(\mathbf{k},\omega) = \frac{-e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\mathbf{q}) - n_F(\mathbf{q}+\mathbf{k})}{\hbar\omega} \left[\frac{1}{1 - \frac{(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})}{\hbar\omega}} \right] \tag{8.20}$$

The leading term in this expansion replaces the square brackets with unity, but then the sum over $\mathbf{q}$ vanishes. For the next term it is useful to write for small $\mathbf{k}$,

$$(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}}) \approx \mathbf{k} \cdot \nabla_{\mathbf{q}} \epsilon^0_{\mathbf{q}}$$

and similarly

$$n_F(\mathbf{q}+\mathbf{k}) - n_F(\mathbf{q}) \approx \mathbf{k} \cdot \nabla_{\mathbf{q}} n_F(\mathbf{q})$$

We thus have

$$\begin{aligned} \chi^0(\mathbf{k},\omega) &= \frac{e}{\mathcal{V}(\hbar\omega)^2} \sum_{\mathbf{q},\sigma} (\mathbf{k} \cdot \nabla_{\mathbf{q}} n_F(\mathbf{q}))(\mathbf{k} \cdot \nabla_{\mathbf{q}} \epsilon^0_{\mathbf{q}}) & (8.21) \\ &= \frac{-e}{\mathcal{V}(\hbar\omega)^2} \left[\sum_{\mathbf{q},\sigma} n_F(\mathbf{q}) \right] \left[(\mathbf{k} \cdot \nabla_{\mathbf{q}})^2 \epsilon^0_{\mathbf{q}} \right] & (8.22) \end{aligned}$$

In obtaining the second line, we have integrated by parts (convert to integral, integrate by parts and convert back to a sum). The quantity in the second square bracket is $\hbar^2 k^2/(m)$ and is $\mathbf{q}$ independent. The quantity in the first square bracket can thus be summed alone to just give N. We thus have in this limit of large ω

$$\chi^0(\mathbf{k}, \omega) = \frac{-ek^2 n}{m\omega^2} \tag{8.23}$$

where n is the electron density. In fact this result is extremely general — independent of many details of the system, as we will see next.

More general f-sum rule approach

The limit can be obtained by invoking the so-called f-sum rule. We return to the primitive integral form of our response function (See Eq. 8.15)

$$\chi(\mathbf{k}, \omega) = \frac{ie}{\hbar \mathcal{V}} \int_0^\infty dt \; e^{i(\omega + i\varepsilon)t} \langle [\hat{n}(\mathbf{k}, t), \hat{n}(-\mathbf{k}, 0)] \rangle$$

Where

$$\hat{n}(\mathbf{k}, t) = e^{iHt/\hbar} \hat{n}(\mathbf{k}) e^{-iHt/\hbar}$$

and here we would like to be completely general, so we consider *any* Hamiltonian H at this point (which may include electron-electron interactions, for example).

Since we are interested in high frequency, we equivalently want to look at small times t. Thus we expand for small t to write

$$\hat{n}(\mathbf{k}, t) \approx \hat{n}(\mathbf{k}) + \frac{it}{\hbar}[H, \hat{n}(\mathbf{k})] + \ldots$$

so that we have[10]

$$\chi(\mathbf{k}, \omega) = \frac{ie}{\hbar \mathcal{V}} \int_0^\infty dt \; e^{i(\omega + i\varepsilon)t} \; \frac{it}{\hbar} \langle [[H, \hat{n}(\mathbf{k}, t)], \hat{n}(-\mathbf{k}, 0)] \rangle$$

This double commutator is familiar from our discussion of the Feynman theory of superfluids. In Eq. 5.11 we discovered that this double commutator is *independent of interactions between particles* and yields the constant $\hbar^2 \mathbf{k}^2 N/m$. Thus we can perform the integral to obtain the same result

$$\chi = \frac{-ek^2 n}{m\omega^2} \tag{8.24}$$

---

[10] The term $\langle [n(\mathbf{k}), n(-\mathbf{k})] \rangle$ has to give zero for a rotationally invariant ground state.

Drude Theory Approach

In fact one can get the same result out of simple Drude theory for a translationally invariant system. Translational invariance here means there should be no scatterers. Let us start with the current conservation equation (with the overdot being time derivative)

$$\dot{\delta n}(\mathbf{r}, \mathbf{t}) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0$$

where here δn is the local change in particle density and $\mathbf{j}$ is the local particle current. Let us rewrite this in terms of its frequency and wavevector Fourier modes

$$-i\omega\, \delta n(\mathbf{k}, \omega) + i\, \mathbf{k} \cdot \mathbf{j}(\mathbf{k}, \omega) = 0$$

which we can write as

$$j_{\parallel} = \frac{\omega\, \delta n}{k} \tag{8.25}$$

We can then use the equations of motion when an electric field is applied

$$m\dot{\mathbf{v}} = -e\mathbf{E}$$

where the velocity is related to the current density by

$$\mathbf{j} = \bar{n}\mathbf{v}$$

with $\bar{n}$ the average density[11]. We thus have

$$m\dot{\mathbf{j}} = -e\bar{n}\mathbf{E} = e\bar{n}\nabla\phi$$

again moving to Fourier space we have

$$-i\omega m j_{\parallel}(k, \omega) = ie\bar{n}k\ \phi(k, \omega)$$

Plugging in Eq. 8.25 we obtain

$$\delta n(\mathbf{k}, \omega) = \frac{-k^2\bar{n}e}{m\omega^2}\ \phi(\mathbf{k}, \omega)$$

8.4 Response of Interacting Electrons: RPA

In the last section we have been considering non-interacting electrons. We have the charge density response to an applied potential

$$\delta n(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, \omega)\phi_{ext}(\mathbf{q}, \omega)$$

---

[11] We would also have a term $\delta n\mathbf{v}$ but this is order $(small)^2$, since both δn and $\mathbf{v}$ are assumed small.

where the superscript 0 indicates noninteracting. We would like to put the interactions back into the system in the simplest way possible. What do the interactions do? Well, if a nonuniform density δn occurs, this will induce a Coulomb interaction

$$\phi_{induced}(\mathbf{r},t) = \int d\mathbf{r}' V(\mathbf{r}-\mathbf{r}')\delta n(\mathbf{r}',t) \tag{8.26}$$

where we will assume here that the interaction V is of Coulomb form

$$V(r) = \frac{-e}{4\pi\epsilon_0 r}$$

although our approach will work for any form of V.

Equation 8.26 is a convolution so we can write it more simply in Fourier space

$$\phi_{induced}(\mathbf{q},\omega) = \tilde{V}(\mathbf{q})\delta n(\mathbf{q},\omega) \tag{8.27}$$

where $\tilde{V}$ is the Fourier transform of $V(\mathbf{r})$.

Now the system must respond to both the externally applied ϕ_{ext} and the induced $\phi_{induced}$. A simple approximation is to assume the system responds like a noninteracting system — and let the entire effect of the interaction be included in the fact that we let the system respond to both the external and the induced potentials. Thus we write

$$\begin{aligned}\delta n(\mathbf{q},\omega) &= \chi^0(\mathbf{q},\omega)\left[\phi_{ext}(\mathbf{q},\omega) + \phi_{induced}(\mathbf{q},\omega))\right] \\ &= \chi^0(\mathbf{q},\omega)\left[\phi_{ext}(\mathbf{q},\omega) + \tilde{V}(\mathbf{q})\delta n(\mathbf{q},\omega))\right]\end{aligned}$$

We can then solve this to obtain

$$\delta n(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1-\chi^0(\mathbf{q},\omega)\tilde{V}(\mathbf{q})}\;\phi_{ext}(\mathbf{q},\omega)$$

or equivalently

$$\delta n(\mathbf{q},\omega) = \chi^{RPA}(\mathbf{q},\omega)\phi_{ext}(\mathbf{q},\omega)$$

where

$$\chi^{RPA}(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1-\chi^0(\mathbf{q},\omega)\tilde{V}(\mathbf{q})} \tag{8.28}$$

This approximation of the response function of an interacting system is known as the RPA approximation[12] or time-dependent self-consistent Hartree approximation, since we are simply treating the effect of the interaction as being an effective potential (Eq. 8.26) that the electrons respond to, analogous to the Hartree approximation we used previously in section 7.3.1.

---

[12] RPA stands for "Random Phase Approximation". However these words mean almost nothing now. The approximation was first used by Bohm and Pines in 1952, and it was derived in a very roundabout way which is no longer used. In that language it was related to random phases, but this is only of historical interest.

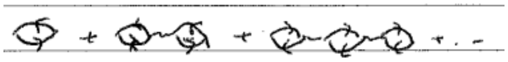

Figure 8.5: The RPA diagrams or bubble sum

One way of understanding the RPA approximation is to expand the denominator and write

$$\chi^{RPA} = \chi^0 + \chi^0 \tilde{V} \chi^0 + \chi^0 \tilde{V} \chi^0 \tilde{V} \chi^0 + \ldots$$

which is shown in diagrammatic language in Fig. 8.5. The physical interpretation of this series is as follows: In the first term, χ^0, the electrons directly respond to the external perturbation. In the second term, $\chi^0 \tilde{V} \chi^0$ the electrons responsd to the perturbation and build up a density which creates a potential and then the electrons respond to this potential. And so forth.

8.4.1 Relation to Dielectric Constant

The response function χ is closely related to the relative dielectric constant. Recall that

$$\mathbf{E} = \frac{1}{\epsilon_r} \mathbf{D}$$

meaning that[13]

$$\phi_{total} = \frac{1}{\epsilon_r} \phi_{ext}$$

But we have

$$\begin{aligned} \phi_{total} &= \phi_{ext} + \phi_{induced} \\ &= \left[1 + \tilde{V} \chi \right] \phi^{ext} \end{aligned}$$

This equation is exact, so long as one uses the exact response function χ in the equation. So we have the exact result

$$\epsilon_r = \frac{1}{1 + \tilde{V} \chi}$$

Note that ϵ_r in principle depends on frequency and wavevector.

Using the RPA approximation for χ we substitute in to obtain

$$\epsilon_r = \frac{1}{1 + \tilde{V} \frac{\chi^0}{1 - V \chi^0}} = 1 - V \chi^0 \tag{8.29}$$

---

[13] Recall that **D** is the field applied normal externaly to a material, whereas **E** is the physical field.

Static Limit

It is useful to look a the static $\omega = 0$ limit. Recall that in this limit (Eq. 8.2)

$$\chi^0 = eD(E_F)$$

and we have the Coulomb interaction in Fourier space (Eq. 7.39)

$$\tilde{V}(k) = \frac{-e}{\epsilon_0 k^2}$$

We thus plug into Eq. 8.29 to get

$$\epsilon_r(\mathbf{k}) = 1 + \frac{e^2}{\epsilon_0 k^2} D(E_F) = 1 + \frac{k_{TF}^2}{k^2}$$

where k_{TF} is the Thomas-Fermi wavevector, Eq. 8.4.

We can then try to find out what happens if we insert a test charge of charge Q into our system. We then have

$$\phi_{ext}(\mathbf{k}) = \frac{Q}{\epsilon_0 k^2}$$

which gives us

$$\phi_{total}(\mathbf{k}) = \frac{1}{\epsilon_r}\phi_{ext} = \frac{Q/\epsilon_0}{k_{TF}^2 + k^2}$$

Fourier transforming this immediately gives

$$\phi_{total}(\mathbf{r}) = \frac{Q}{4\pi\epsilon_0 |\mathbf{r}|} e^{-k_{TF}|\mathbf{r}|} \tag{8.30}$$

matching the Yukawa form we derived in Eq. 8.5.

8.4.2 High Frequency, Low k response: Plasmons

Let us consider interactions in the small k high frequency limit. As we derived above (in several ways!) we have the noninteracting response (Eq. 8.23) given by

$$\chi^0 = \frac{-e\bar{n}k^2}{m\omega^2}$$

If we plug this into the RPA equation (Eq. 8.28) we discover that the denominator $1 - \tilde{V}\chi^0$ diverges when

$$1 = \tilde{V}\chi^0 = \frac{e}{\epsilon_0 k^2} \frac{e\bar{n}k^2}{m\omega^2}$$

or

$$\omega = \sqrt{\frac{e^2 n}{\epsilon_0 m}}$$

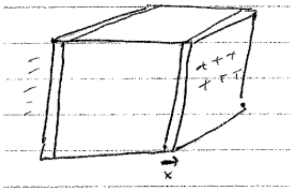

Figure 8.6: Displacing all of the mobile charges by a distance x builds up a surface charge $\rho_{surface} = \bar{n}xe$.

The divergence in χ indicates an excitation mode of the system — in other words, the system responds at finite amplitude to even an infinitessimly small amplitude perturbation if you perturb it in resonance with the excitation energy. This particular excitation mode is known as *plasma oscillation* or *plasmon* (when we think of it as a quantized object like a phonon or photon).

There is actually a very simple physical explanation for the plasmon. We consider a big cube of our material — with mobile negative charges and a stationary positive background. Now let us imagine moving all of our negative charge a distance x in the x direction. This builds up a charge on the two x faces of our cube as shown in Fig. 8.6. The surface charge density that is built up is $\bar{n}xe$. We thus have a capacitor formed by the two charged faces. We may recall that from Gauss' law $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ we can obtain the electric field from a capacitor

$$\mathbf{E} = \rho/\epsilon_0 = \bar{n}xe/\epsilon_0$$

The electric field then applies a force

$$\mathbf{F} = -e\rho/\epsilon$$

to all of the electrons. Newtons law then gives us

$$m\ddot{x} = -e\rho/\epsilon_0 = \frac{-\bar{n}e^2}{\epsilon_0}x$$

thus resulting in harmonic motion with frequency

$$\omega = \sqrt{\frac{e^2 n}{\epsilon_0 m}}.$$

It is important to note that this result holds with the mass m not being renormalized by any interactions (We discussed mass renormalization in the previous chapter, but that does not matter here). The reason the mass remains unrenormalized is because the plasma frequency describes the motion of the center of mass of all of the electrons in the system, and this is completely independent from the details of interaction between electrons. This is quite related to the argument leading up to Eq. 8.24, that the high frequency response is unchanged by interactions between particles.

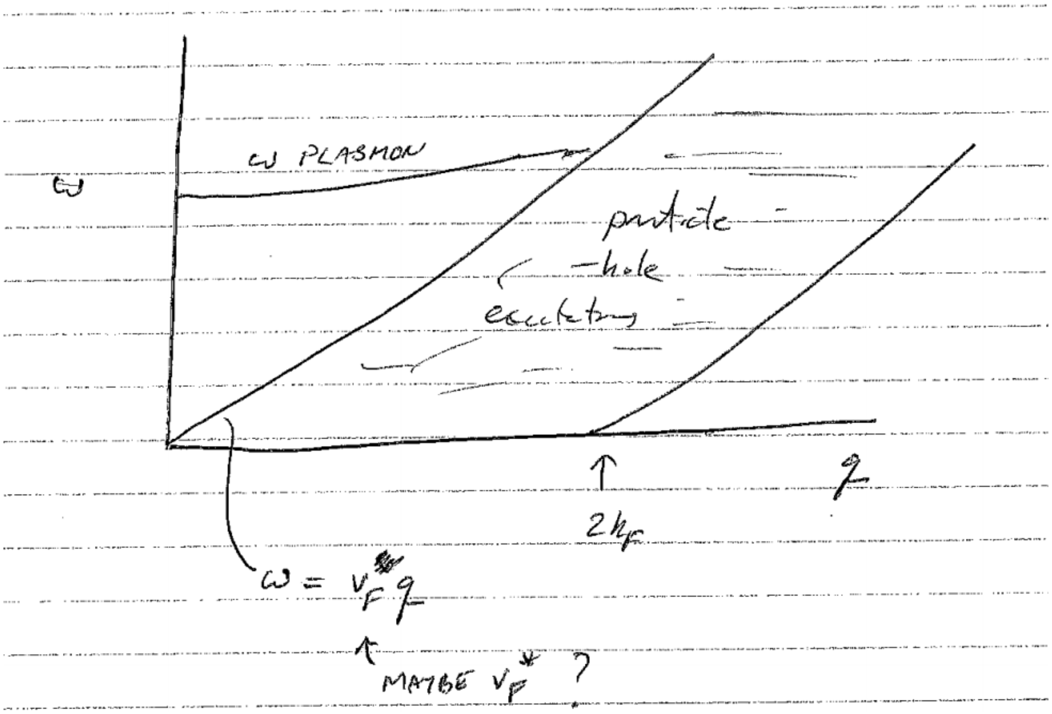

Figure 8.7: The excitation spectrum of an electron gas in three dimensions, with Coulomb interaction between particles. This is qualitiatively similar to Fig. 8.4 except that the Coulomb interaction gives an isolated plasma mode at small k and high frequency. In RPA calculation, the upper edge of the particle-hole excitation band is at $\omega = v_F q$ with v_F the unrenormalized Fermi velocity. However, in more detailed calculations this will be modified to $\omega = v_F^* q$ with a renormalized effective mass. However, the frequency of the plasma mode remains unrenormalized.

In Fig. 8.7 we sketch the excitation spectrum of a three dimensional electron gas with Coulomb interactions. The spectrum is qualitatively similar to the noninteracting fermion spectrum shown in Fig. 8.4 except for the addition of the plasma mode at $\omega_{plasmon}$ at small wavevector k. In the RPA calculation, the upper edge of the particle-hole excitation band is at $\omega = v_F q$ with v_F the unrenormalized Fermi velocity. In a more detailed calculation this will be modified to $\omega = v_F^* q$ with a renormalized effective mass. However, the frequency of the plasma mode remains unrenormalized.

8.5 Chapter Appendix: Deriving Lindhard Screening expression

We start with Eq. 8.16. Making use of inversion symmetry of the system we have $\chi(\mathbf{k},\omega) = \chi(-\mathbf{k},\omega)$ so we can write

$$\begin{aligned}
\chi(\mathbf{k},\omega) &= \frac{-e}{\hbar\mathcal{V}}\sum_m \left\{ \frac{|\langle \mathrm{GS}|\hat{n}(-\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_m - E_{\mathrm{GS}})/\hbar} - \frac{|\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_{\mathrm{GS}} - E_m)/\hbar} \right\} \\
&= \frac{-e}{\hbar\mathcal{V}}\sum_m \left\{ \frac{|\langle m|\hat{n}(\mathbf{k})|\mathrm{GS}\rangle|^2}{\omega + i\varepsilon - (E_m - E_{\mathrm{GS}})/\hbar} - \frac{|\langle m|\hat{n}(-\mathbf{k})|\mathrm{GS}\rangle|^2}{\omega + i\varepsilon - (E_{\mathrm{GS}} - E_m)/\hbar} \right\} \qquad (8.31)
\end{aligned}$$

Conisder the first term in the brackets of Eq. 8.31. Writing

$$\hat{n}(\mathbf{k}) = \sum_{\mathbf{q},\sigma} c^\dagger_{\mathbf{q}+\mathbf{k},\sigma} c_{\mathbf{q},\sigma}$$

the intermediate state is clearly $|m\rangle = c^\dagger_{\mathbf{q}+\mathbf{k},\sigma} c_{\mathbf{q},\sigma}|\mathrm{GS}\rangle$. We can thus write the first term of the sum as

$$\frac{-e}{\hbar\mathcal{V}}\sum_{\mathbf{q},\sigma} \frac{\Theta(|\mathbf{q}+\mathbf{k}| > k_F)\,\Theta(|\mathbf{q}| < k_F)}{\omega + i\epsilon - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{q}})/\hbar} \qquad (8.32)$$

with Θ the step function.

Similarly consider the second term in the brackets of Eq. 8.31. The intermediate state is $|m\rangle = c^\dagger_{\mathbf{q}-\mathbf{k},\sigma} c_{\mathbf{q},\sigma}|\mathrm{GS}\rangle$. So we can write the second term in the sum as

$$\frac{e}{\hbar\mathcal{V}}\sum_{\mathbf{q},\sigma} \frac{\Theta(|\mathbf{q}-\mathbf{k}| > k_F)\,\Theta(|\mathbf{q}| < k_F)}{\omega + i\epsilon - (\epsilon_{\mathbf{q}} - \epsilon_{\mathbf{q}-\mathbf{k}})/\hbar}$$

In this second term we now shift summation variables $\mathbf{q} \to \mathbf{q} + \mathbf{k}$. So the term becomes

$$\frac{e}{\hbar\mathcal{V}}\sum_{\mathbf{q},\sigma} \frac{\Theta(|\mathbf{q}| > k_F)\,\Theta(|\mathbf{q}+\mathbf{k}| < k_F)}{\omega + i\epsilon - (\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{q}})/\hbar}$$

Summing this with Eq. 8.32 yields

$$\chi(\mathbf{k},\omega) = \frac{-e}{\hbar\mathcal{V}}\sum_{\mathbf{q},\sigma} \frac{\Theta(|\mathbf{q}+\mathbf{k}| > k_F)\,\Theta(|\mathbf{q}| < k_F) - \Theta(|\mathbf{q}| > k_F)\,\Theta(|\mathbf{q}+\mathbf{k}| < k_F)}{\omega + i\epsilon - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{q}})/\hbar}$$

This form is equivalent to that of Eq. 8.18 except that the numerators look differnt. By looking at all four cases where $|\mathbf{q}|$ is greater or less than k_f and $|\mathbf{q}+\mathbf{k}|$ is greater or less than k_F it is easy to see that these numerators are in fact identical, thus completing the calculation.

Chapter 9

Landau Fermi Liquid Theory

9.1 Background

What we have done so far (first order perturbation theory, Hartree-Fock, RPA) is fairly accurate for weakly interacting Fermi systems. However, real physical fermion systems usually have strong interactions[1]. Whether we are talking about metals, ^{3}He, neutron stars, or semiconductors[2], we typically have the interaction larger than the Fermi energy

$$E_{interaction} > E_F$$

As a result the calculations we have done so far cannot be used quantitatively[3], although they can be used for qualitative inspiration. Despite this strong warning, we almost always get away with ignoring interactions completely. Indeed, almost all of semiconductor physics (including the whole semiconductor industry) is built on the idea of mostly non-interacting electrons. Why does this make any sense at all? I'm glad you asked!

Understanding of strongly interacting fermions really began with experiments on ^{3}He. This system is much simpler than systems of electrons because of the absence of long ranged Coulomb interactions. In 1953-1954, William Fairbank[4] manged to cool ^{3}He to below about 1K which is less than the Fermi energy $E_F \approx 5$K. At low temeperature he

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[1] In recent years people have been able to make cold atomic Fermi gases where one can tune the interaction strength, and almost turn it off if desired. A huge amount of the pioneering research on cold fermionic atomic systems was done by Debbie Jin, who very sadly died of cancer at the young age of 47 in 2016.

[2] One might think that the low density of semiconductors might help. However, this turns out not to be true. The interaction is on the scale of $e^2/(\epsilon a)$ where a is the distance between fermions, whereas the kinetic energy is on the scale $\hbar^2/(2ma^2)$, so as we make the density lower, in fact the ratio of interaction to Fermi energy actually increases!

[3] There is an exception: At small enough q and high enough ω, RPA becomes exact even for strongly interacting systems.

[4] Fairbank was at Duke university at the time (where he recruited Fritz London in 1952). A few milligrams of ^{3}He was supplied by Oak Ridge National Lab, where much of the research for the American nuclear project was being done. This small amount was plenty for conducting the key experiments.

was able to see evidence of the Fermi-Dirac distribution. In particular, he measured

$$\begin{aligned} C_v &\sim T \\ \chi &\sim \text{indep of } T \end{aligned}$$

where here χ means the pauli paramagnetic susceptibility (and as usual C_v is heat capacity). Both of these relations are indicative of fermions. However, in both cases, the proportionality constants did not match the predictions of the noninteracting fermion model. Now in our discussion of Hartree-Fock approximation above, we already have seen that the particle mass can be renormalized by interactions. However, this alone does not fix the problem in a consistent manner[5]. .

9.2 Basics Idea of Fermi Liquid Theory

In 1956, Landau, in one of his classic papers[6], explained how we should understand interactions of fermions. This work, based on brilliant intuition, set the language for our understanding of Fermions, and was fully justified many years later using both perturbation theory and renormalization group methods.

9.2.1 Landau's Conjecture

Landau conjectured that interacting fermions should be just like noninteracting fermions, but "dressed" by interactions. What he meant by this is that

- The ground state shold be a "dressed" Fermi sea
- Low energy excitations, can be described in terms of *quasiparticle* excitations of the ground state. These are "dressed" versions of the noninteracting excitations of the Fermi sea.

The key question here is what we mean by "dressed". Here we mean that it needs to include a cloud of interactions with its surroundings. This very vague statement we will make more definite by the following argument:

Landau Adiabaticity Argument

Let us imagine starting with the noninteracting case adiabatically turning on the interactions. Since this is a procedure that can be implimented using a Hamiltonian that we

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[5] If one were to try to just replace the mass with an effective mass, one would require two different effective masses to explain the two different experiments!

[6] Titled, "The Theory of Fermi Liquids". This is a rather remarkable paper. It is only 6 pages long and has only a single citation (to the experiment by Fairbank).

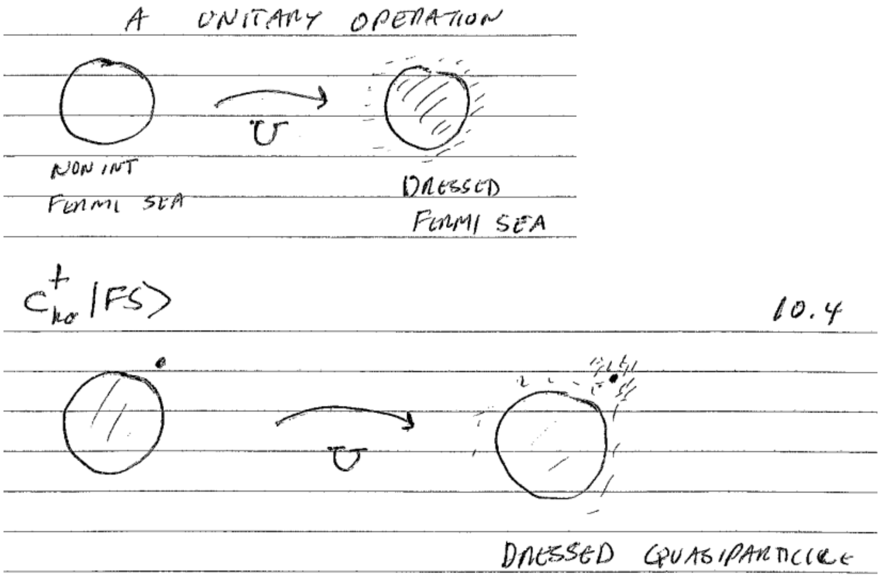

Figure 9.1: Top: turning on interaction adiabatically turns a noninteracting Fermi sea into the interacting "dressed" ground state. Bottom: If we start with a Fermi sea plus a single particle outside the Fermi sea, when we turn on the interaction, we obtain a *quasiparticle*.

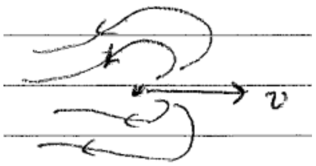

Figure 9.2: Fluid backflow around a moving object.

modify in time, it must be representable using a unitary (time evolution) operator. The result of this procedure gives the dressed Fermi sea. This is depicted as a cartoon in the top of Fig. 9.1. Similarly, we can start with a single fermion added to the noninteracting Fermi sea and adiabatically turn on the interaction. Here we get a dressed Fermi sea with a dressed additional particle outside of the Fermi sea as shown in the bottom of Fig. 9.1. We call this dressed additional particle a *quasiparticle*.

Here it is key to realize that in turning on the interaction, the quantum numbers of the system do not change — in particular, the momentum and spin are unchanged. Thus the dressed quasiparticles are in one-to-one correspondence with the noninteracting particles. However, in contrast to the noninteracting particles, the quasiparticles carry with them a cloud of interactions with their environment. This is very much like the idea of backflow around a moving object in a fluid as shown in Fig. 9.2.

Why does this picture of dressed quasiparticles make sense? To answer this we should ask the opposite question: how could this picture fail? (Of course one could always

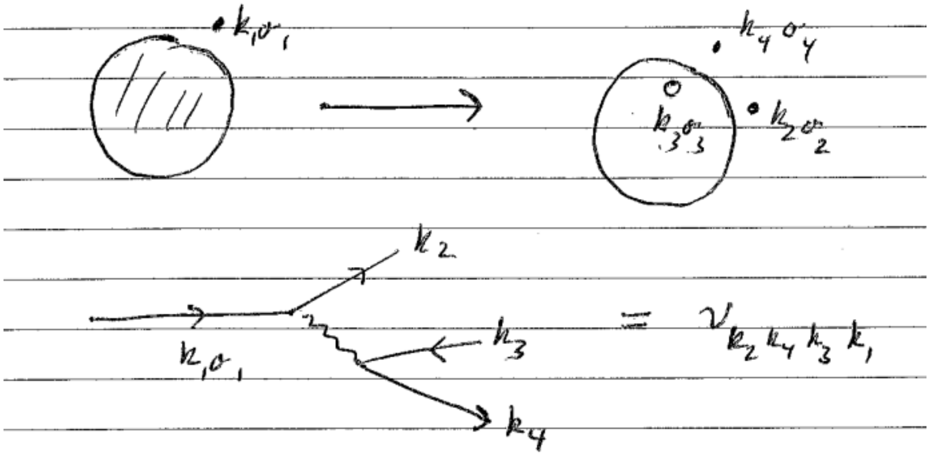

Figure 9.3: Two different depictions of quasiparticle decay of a single particle added above a Fermi surface.

have a first order transition when the interaction turns on and the new ground state could be something completely different, like a crystal, but let us assume that such a first order transition does not occur.) The only way our picture of dressed particles can fail is if the introduction of interactions lets the quasiparticle decay into multiple other quasiparticles — then the idea that we have a "single-particle" excitation will fail.

Let us think about what would have to be the case if such a decay were to happen. Of course we need to conserve both energy and momentum. If we have an initial momentum of our additional particle is $\mathbf{k}_1$ above the Fermi surface ($|\mathbf{k}_1| > k_F$), we can imagine that it decays into two quasipartcles with momenta $\mathbf{k}_2, \mathbf{k}_4$ above the Fermi surface and a quasihole with momentum $\mathbf{k}_3$ below the Fermi surface. Such a process is shown in Fig. 9.3.

The key claim here is that due to phase space restrictions associated with energy conservation, the scattering lifetime for such a process is

$$\tau \sim |k_1 - k_F|^{-2} \tag{9.1}$$

so if we are considering quasielectrons or quasiholes very close to the Fermi surface, they are very long lived, i.e., they do not fall apart. If a particle is "close enough" to the Fermi surface it lives essentially forever, meaning it is in an eigenstate.

Here is a quasiproof of the statement Eq. 9.1. In the process shown in Fig. 9.3, all of the particles have energy $v_F|k - k_F|$ with their given k, independent of whether they are quasiparticles or quasiholes (a quasihole below the Fermi surface costs positive energy). We then enforce that the intitial energy must be the same as the final energy, so that in calculating the scattering rate using Fermi's golden rule we will have integrals of the form

$$\frac{1}{\tau} \sim \int_0^\infty d\epsilon_2 \int_0^\infty d\epsilon_3 \int_0^\infty d\epsilon_4 \;\; \delta(\epsilon_1 - (\epsilon_2 + \epsilon_3 + \epsilon_4))$$

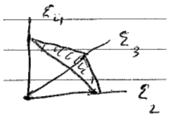

Figure 9.4: The region that conserves energy is the area of triangular piece of a plane a distance ϵ_1 out along each axis.

where ϵ_1 is the initial energy and $\epsilon_2, \epsilon_3, \epsilon_4$ are the three final energies of the three final particles. As shown in Fig. 9.4 the value of this integral is equal to the area of a triangular region in $(\epsilon_2, \epsilon_3, \epsilon_4)$ space which intersects each axis at a value ϵ_1. Thus we obtain

$$\text{Area} \sim \epsilon_1^2 \sim |k_1 - k_F|^2$$

Thus the scattering rate decreases as we approach the Fermi surface and we have well defined quasiparticles[7].

9.3 Properties of the Dressed Fermi Liquid

Let us then ask what the dressing of the Fermi liquid looks like in more detail. As written figuratively in Fig. 9.1, the dressing is given by some unitary transformation U. So that the interacting ground state can be written in terms of the noninteracting ground state

$$|\text{GS}\rangle = U|\text{GS}^0\rangle$$

Similarly we can write creation operators for the dressed quasiparticles $\tilde{c}^\dagger_{\mathbf{k},\sigma}$ by dressing the noninteracting quasiparticles $c^\dagger_{\mathbf{k},\sigma}$

$$\tilde{c}^\dagger_{\mathbf{k},\sigma} = U c^\dagger_{\mathbf{k},\sigma} U^\dagger$$

Now notice that the occupation of these dressed quasiparticles in the ground state is simply a step function, since

$$\begin{aligned} n^{qp}(\mathbf{k},\sigma) &= \langle \hat{n}_{qp}(\mathbf{k},\sigma)\rangle = \langle \text{GS}|\tilde{c}^\dagger_{\mathbf{k},\sigma}\tilde{c}_{\mathbf{k},\sigma}|\text{GS}\rangle \\ &= \langle \text{GS}^0|U^\dagger U \tilde{c}^\dagger_{\mathbf{k},\sigma} U^\dagger U \tilde{c}_{\mathbf{k},\sigma} U^\dagger U|\text{GS}^0\rangle \\ &= \langle \text{GS}^0|c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}|\text{GS}^0\rangle = n_F(k) \end{aligned}$$

It is much more complicated to find the occupancy of the *noninteracting* plane wave orbitals in the *interacting* ground state. Generally, this will be a hard task. However, at

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[7] There has recently been a lot of study of so-called non-Fermi liquid cases where the quasiparticle is not well defined because $1/\tau > \epsilon$. Certain models of high temperature superconductors have this property, for example.

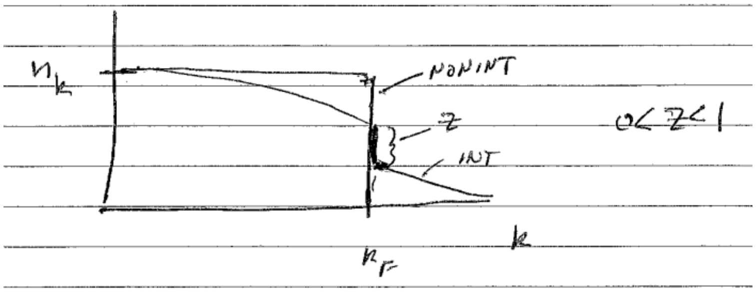

Figure 9.5: An interacting Fermi liquid still has a step in the occupation at k_F, although the step is not as big as for a noninteracting Fermi system.

least if the interaction is weak, we can apply perturbation theory to write the interacting ground state in terms of the noninteracting one:

$$\begin{aligned} |\mathrm{GS}\rangle &= \eta \left[|\mathrm{GS}^0\rangle + \sum_{n \neq GS} \frac{|n\rangle\langle n|V|\mathrm{GS}^0\rangle}{E_n - E_{GS}} + \ldots \right] \qquad (9.2) \\ &= \eta \left[|\mathrm{GS}^0\rangle + \sum_{\mathbf{q}_1,\mathbf{q}_2 > k_F; \mathbf{q}_3,\mathbf{q}_4 < k_F} c^\dagger_{\mathbf{q_1}} c^\dagger_{\mathbf{q_2}} c_{\mathbf{q_4}} c_{\mathbf{q_3}} |\mathrm{GS}^0\rangle \frac{v_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4}}{E_{\mathbf{q}_1} + E_{\mathbf{q}_2} - E_{\mathbf{q}_3} - E_{\mathbf{q}_4}} + \ldots \right] \end{aligned}$$

where η is a factor included to keep the wavefunction properly normalized (and we have dropped spin indices for simplicity).

Now when we calculate the occupation of the original orbitals we have

$$\begin{aligned} n(\mathbf{k},\sigma) &= \langle \hat{n}(\mathbf{k},\sigma) \rangle = \langle \mathrm{GS}| c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} |\mathrm{GS}\rangle \\ &= \langle \mathrm{GS}^0 | U^\dagger c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} U | \mathrm{GS}^0 \rangle \end{aligned}$$

and the unitary transform is precisely the series shown in Eq. 9.2. The key thing to note here is that, at least perturbatively, there must remain a step in the occupation $n(k)$ coming from the first term in the series. It is a less pronounced step than for a purely noninteracting system, but it is a step nonetheless as shown in Fig. 9.5.

This brings us to an important fact about interacting Fermi systems. (We can even generalize our consideration now to arbitrary band structures in crystals, not just simple spherically symmetric systems).

Let us define a Fermi surface to be the locus of points in k-space where there is a discontinuity in $\hat{n}(\mathbf{k})$.

Luttinger's Theorem:[8] The volume of the Fermi sea in k-space is unchanged by interactions.

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[8] Joaquin (Quin) Mazdak Luttinger discovered this (partially with John Ward) in 1960. Those who know field theory know Ward from the famous Ward identities, which are key to the derivation of this theorem.

In a rotationally invariant system, this means k_F is unchanged by interactions.

9.4 Landau Free Energy Functional

Given this quasiparticle concept, how are we going to describe the physics of a Fermi liquid. The general idea is to always describe a system by the occupation of the quasiparticle states $n_{\mathbf{p},\sigma}$. (Above we called this $n^{qp}(\mathbf{k},\sigma)$ to distinguish it from the noninteracting particle occupation. Here we will drop the qp and also write this as a function of $\mathbf{p}$ rather than $\mathbf{k}$ as is more conventional in the field.) Remember that we are describing the quasiparticle occupancy here!

As mentioned above, at $T=0$ we expect to have the usual step function occupancy

$$T=0 \qquad n^0_{\mathbf{p},\sigma} = \left\{ \begin{array}{ll} 1 & |\mathbf{p}| < p_F \\ 0 & |\mathbf{p}| > p_F \end{array} \right.$$

The superscript 0 means this is the occupancy in equilibrium (i.e., unperturbed). At finite temperature we would have a Fermi function instead of a step function.

Let us now consider small perturbations to this distribution such that any excited quasiparticle or quasihole stays near the Fermi surface. We can then Taylor expand

$$\delta n_{\mathbf{p},\sigma} = n_{\mathbf{p},\sigma} - n^0_{\mathbf{p},\sigma}$$

We the expect the change of free energy to be given by

$$\mathcal{F} - \mathcal{F}_0 \approx \sum_{\mathbf{p},\sigma} (\epsilon_p - \mu)\delta n_{\mathbf{p},\sigma} + \ldots$$

Since we are near the Fermi surface we have

$$\epsilon_{\mathbf{p}} - \mu = v^*_F(|\mathbf{p}| - p_F)$$

where we have linearized around the Fermi surface. Note in particular that we are using the effective mass here

$$v^*_F = p_F/m^*$$

which tells us the energy of a single quasiparticle above (or below) the Fermi surface. Here our intuition is from Hartree-Fock, where we learned that the effective mass of a particle can be renormalized by interactions.

A key realization by Landau is that the energy difference $F - F_0$ is second order in small quantities: Both $|\mathbf{p}| - p_F$ is small and δn is also small. As a result, to be consistent, we must consider other terms of roughly the same size — i.e., the next terms in the Taylor expansion giving

$$\mathcal{F} - \mathcal{F}_0 = \sum_{\mathbf{p},\sigma} (\epsilon_p - \mu)\delta n_{\mathbf{p},\sigma} + \frac{1}{2} \sum_{\mathbf{p},\mathbf{p}',\sigma,\sigma'} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')\delta n_{\mathbf{p},\sigma}\delta n_{\mathbf{p}',\sigma'} + \ldots \qquad (9.3)$$

The quantity $f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')$ is some arbitrary interaction between a quasiparticle with momentum $\mathbf{p}$ with spin σ and another quasiparticle with momentum $\mathbf{p}'$ with spin σ'. What is crucial here is that this allows for a shift in energy, but it does not allow for scattering — i.e, changing momentum! (The reason for this being the idea that the quasiparticle is very close to being an eigenstate when it is near the Fermi surface).

Aside: We've been thinking in terms of spins σ which can be $\uparrow$ or $\downarrow$. However, more generally we would have to consider cases when the spin is polarized in the x-direction. As such we would write a density matrix $\delta n_{\alpha,\beta}(\mathbf{p})$ rather than just a density. So for example, the spin of the quasiparticle would be

$$\langle \overrightarrow{s} \rangle = \mathrm{Tr}[\overrightarrow{\sigma}_{\beta,\alpha}\delta n_{\alpha,\beta}]$$

and the interaction function would be a more complicated $f_{\alpha,\beta;\gamma,\delta}(\mathbf{p},\mathbf{p}')$. Fortunately, we will never need to deal with this more complicated situation. **end of aside**

Differentiating Eq. 9.3 we can obtain the energy of a quasiparticle $\tilde{\epsilon}$ when it is in the presence of other quasiparticles

$$\frac{\delta F}{\delta n_{\mathbf{p}}} = \tilde{\epsilon}_{\mathbf{q},\sigma} - \mu = \epsilon_{\mathbf{p}} - \mu + \sum_{\mathbf{p}',\sigma'} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')\delta n_{\mathbf{p}',\sigma'}$$

The term including f here gives the energy shift of the quasiparticle due to the presence of other quasiparticles!

We now implement a number of simplifications.

1. We assume $\mathbf{p}$ and $\mathbf{p}'$ are both near the Fermi surface, so that

   $$f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') = f_{\sigma,\sigma'}(\hat{\mathbf{p}},\hat{\mathbf{p}}')$$

   with $\hat{\mathbf{p}}$ being the direction of $\mathbf{p}$.

2. Further assuming rotational invariance we have

   $$f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') = f_{\sigma,\sigma'}(\theta_{\hat{\mathbf{p}},\hat{\mathbf{p}}'})$$

   with θ being the angle between $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$.

   We can then further decomposte f into harmonics

   $$\begin{aligned} f_{\sigma,\sigma'}(\theta) &= \sum_{l\geqslant 0} f_{l,\sigma,\sigma'} P_l(\cos\theta) \\ f_{l,\sigma,\sigma'} &= \frac{2l+1}{2}\int_{-1}^{1} P_l(\cos\theta) f_{\sigma,\sigma'}(\theta)\ d\cos\theta \end{aligned}$$

   where P_l is the Legendre polynomial.

   In particular, this implies

   $$f_{0,\sigma,\sigma'} = \frac{1}{4\pi}\int_{sphere} d\hat{\Omega}\, f_{\sigma,\sigma'}(\theta_{\hat{\Omega}})$$

3. We further assume our system is spin rotationally invariant this means that

$$\begin{aligned} f_{l,\uparrow\uparrow} &= f_{l,\downarrow\downarrow} \\ f_{l,\uparrow\downarrow} &= f_{l,\downarrow\uparrow} \end{aligned}$$

So that it is convenient to define the symmetric and antisymmetric combinations

$$\begin{aligned} f_l^s &= \frac{1}{2}\left(f_{l,\uparrow\uparrow} + f_{l,\uparrow\downarrow}\right) \\ f_l^a &= \frac{1}{2}\left(f_{l,\uparrow\uparrow} - f_{l,\uparrow\downarrow}\right) \end{aligned}$$

Finally we note that f has dimensions of energy (everything else in the least term of Eq. 9.3 is dimensionless). It is then convenient to define a dimensionless quantity. Let us define the density of states

$$D^*(\epsilon_F) = \frac{\mathcal{V} m^* p_F}{\hbar^3 \pi^2}$$

Note that this quantity has dimensionsl of 1/energy, and represents the density of states for quasiparticles (having a factor of m^* in it rather than m). We can then define the dimensionless quantities

$$F_l^{s,a} = D^*(\epsilon_F) f_l^{s,a}$$

known as Fermi liquid coefficients. These parameters along with m^* and k_F completely describe our Fermi liquid. Note that not all these parameters are completely independent: in particular we will see that m^* is related to F_1^s.

These F_l parameters describe the energy renormalizations associated with making a deformation of the Fermi surface in the shape of the l^{th} spherical harmonic The s superscript means both spin Fermi surfaces are deformed in the same way whereas the a superscript means the two Fermi surfaces are deformed in opposite ways.

Aside: Although the following may look complicated, I think it clarifies a number of issues (Ref: See book by Baym and Pethick). If we write the shape of the deformed surface as

$$\delta p_F(\hat{\mathbf{p}}, \sigma) = p_\sigma P_l(\cos\theta)$$

with θ measured from some given point on the sphere, we get an energy of deformation given by

$$\mathcal{F} - \mathcal{F}_0 \sim p_s^2 \left(1 + \frac{F_l^s}{2l+1}\right) + p_a^2 \left(1 + \frac{F_l^a}{2l+1}\right)$$

where $p_s = p_\uparrow + p_\downarrow$ and $p_a = p_\uparrow - p_\downarrow$. Note the stability condition that $F_l > -(2l+1)$. If this condiditon is violated then the Fermi sea deforms spontaneously in the ground state. **end aside**

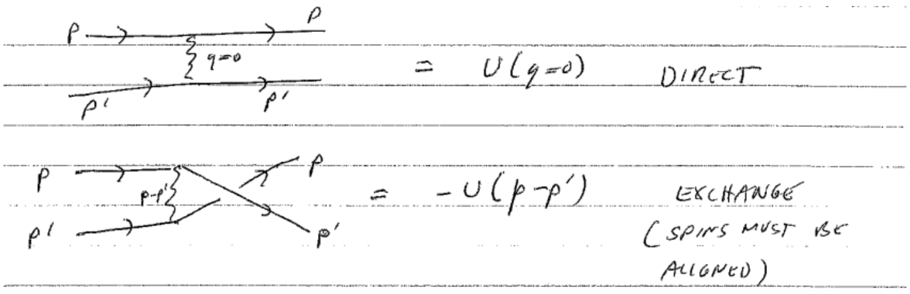

Figure 9.6: The two processes contributing to the interaction energy between $\mathbf{p}$ and $\mathbf{p}'$ included at first order in interaction strength.

Example: f at first order

It is useful to try calculating the function f at first order in the interactions. Recall that $f(\mathbf{p}, \mathbf{p}')$ is the interaction between quasiparticles at $\mathbf{p}$ and $\mathbf{p}'$ but does not allow scattering to another momentum $\mathbf{p}''$. (Again this is the well-defined quasiparticle assumption).

There are two processes in this interaction which we can label direct and exchange, analogous to the interactions we discussed in prior chapters. These two processes are shown in Fig. 9.6. The direct process (as in prior chapters) simply contributes $\tilde{V}(\mathbf{q} = 0)$ (the interaction bewtween two uniform densities). This is independent of the spin state of the two quasiparticles. The more interesting contribution is the exchange term which gives $-\tilde{V}(\mathbf{p} - \mathbf{p}')$, and this contribution requires both spin states to be aligned. Thus we have

$$\begin{aligned} f_{\uparrow,\downarrow}(\mathbf{p}, \mathbf{p}') &= \tilde{V}(0) \\ f_{\uparrow,\uparrow}(\mathbf{p}, \mathbf{p}') &= \tilde{V}(0) - \tilde{V}(\mathbf{p} - \mathbf{p}') = \tilde{V}(0) - \tilde{V}(2p_F \cos\theta_{\mathbf{p},\mathbf{p}'}) \end{aligned}$$

Example: ^{3}He

Examples of the Fermi liquid parameters for ^{3}He are given in the following table (Book Helium 3 by Dobbs)

	m^*/m	F_0^s	F_0^a	F_1^s	F_1^a	F_2^s	F_2^a
1 atm	2.93	11.5	-0.71	5.8	-0.61	-0.18	-0.8
33.5 atm	5.81	87.1	-0.75	14.4	-1.01	0.83	0.0

Note that the F_0^a parameter is close to the stability boundary -1 where it deforms spontaneously in the ground state (in this case meaning that it becomes ferromagnetic, see section 9.5.2 below).

Figure 9.7: To find compressibility we imagine an expansion of the Fermi surface by dp_F

9.5 Results from Fermi Liquid Theory

We are now in a position to use Landau's Fermi liquid theory to calculate some physical responses to small external perturbations.

9.5.1 Compressibility

Let us try to find the compressibility $\partial N/\partial\mu$. changing the number density involves an expansion or compression of the Fermi surface as shown in Fig. 9.7 Let us imagine expanding the Fermi surface by dp_F. We then want to calculate the new chemical potential

$$\begin{aligned}\mu^{new} &= \text{Energy of qp on the new Fermi surface}\\ &= \tilde{\epsilon}_{p_F+dp_F}\\ &= \epsilon_{p_F+dp_F} + \sum_{\mathbf{p}',\sigma} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')\delta n_{\mathbf{p}',\sigma'}\end{aligned}$$

Here we have

$$\epsilon_{p_F+dp_F} = \mu^{old} + v_F^* dp_F$$

with $v_F^* = p_F/m^*$, and in the interaction term we should use

$$\delta n_{\mathbf{p},\sigma} = \begin{cases} 1 & p_F < |\mathbf{p}| < p_F + dp_F \\ 0 & \text{otherwise}\end{cases}$$

representing the change in the Fermi surface. We thus have

$$\mu^{new} = \mu^{old} + v_F^* dp_F + \sum_{p_F<|\mathbf{p}'|<p_F+dp_F,\sigma'} f_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')$$

I.e., the renormalization of the energy at the Fermi surface contains the usual dispersion of energy ($v_F^* dp_F$) plus the change in the interaction term. We can rewrite this as

$$\mu^{new} = \mu^{old} + v_F^* dp_F + \left(\begin{array}{c}\text{number of } p \text{ states}\\ \text{between } p_F \text{ and } p_F + dp_F\end{array}\right)\left[\frac{1}{4\pi}\int d\hat{\Omega}\sum_{\sigma'} f_{\sigma,\sigma'}(\hat{\Omega})\right]$$

The quantity in the square brackets we recognize as $2f_0^s$ and the quantity in the round brackets we recognize as

$$\left(\begin{array}{c}\text{number of } p \text{ states}\\ \text{between } p_F \text{ and } p_F + dp_F\end{array}\right) = \frac{1}{2}D(E_F)v_F dp_F = \frac{1}{2}D^*(E_F)v_F^* dp_F$$

Putting these together and recalling the definition of F_0^s we obtain

$$\frac{\partial \mu}{\partial p_F} = v_F^*(1 + F_0^s)$$

Noninteracting Case: For noninteracting fermions we have

$$\frac{\partial \mu}{\partial p_F} = v_F$$

So the compressibility is

$$\frac{\partial N}{\partial \mu} = \frac{\partial N}{\partial p_F}\frac{\partial p_F}{\partial \mu}$$

and here it is easy to show $\partial N/\partial p_F = D(E_F)v_F$, so we have

$$\frac{\partial N}{\partial \mu} = [D(E_F)v_F]\frac{1}{v_F} = D(E_F)$$

which is what we usually expect.

Interacting case: Here we use instead

$$\frac{\partial \mu}{\partial p_F} = v_F^*(1 + F_0^s)$$

So that

$$\begin{aligned}\frac{\partial N}{\partial \mu} &= \frac{\partial N}{\partial p_F}\frac{\partial p_F}{\partial \mu} \\ &= [D(E_F)v_F]\frac{1}{v_F^*(1 + F_0^s)}\end{aligned}$$

But using the fact that

$$D(E_F)v_F = D^*(E_F)v_F^*$$

we get the final result

$$\frac{\partial N}{\partial \mu} = \frac{D^*(E_F)}{1 + F_0^s}$$

which shows that the compressibility is renormalized both by the expected mass renormalization (resulting in the * on $D^*(E_F)$) but also by the Fermi liquid coefficient F_0^s.

9.5.2 Spin Susceptibility

Here we want to consider a similar expansion/compression of the Fermi surface. However, in this case we let the up spins expand and the down spins compress, corresponding to a net change in magentization, as shown in Fig. 9.8. This is an *spin-antisymmetric* deformation of the Fermi surface, and hence will couple to F_0^a as compared to the spin-symmetric deformation we considered in calculating the compressibility. For noninteracting fermions,

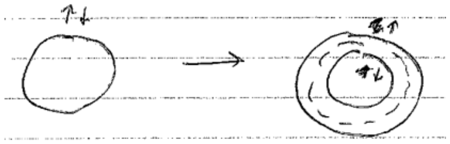

Figure 9.8: To determine spin susceptibility, we increase the size of the Fermi surface for spin up and reduce the size of the Fermi surface for spin down

this gives the usual Pauli spin susceptibility calculation. Yielding the result

$$\chi_{Pauli} = (\frac{1}{2} g \mu_B)^2 \mu_0 D(E_F)$$

with μ_B being the Bohr magneton and g the g-factor. However, with a very similar calculation as we did for compressibility above, we determine the susceptibility for interacting fermions is

$$\chi = (\frac{1}{2} g \mu_B)^2 \mu_0 \frac{D^*(E_F)}{1 + F_0^a}$$

so that the spin susceptibility is again renormalized both by the mass renormalization and the Fermi liquid parameter, F_0^a in this case.

Note that if $F_0^a < -1$ we have $\chi < 0$. This means that it is energetically favorable[9] for the ground state to deform by making a spin-antisymmetric deformation of the Fermi surface — i.e., the Fermi surface spontaneously magnetizes and we have a ferromagnet!

9.5.3 Mass Renormalization

Since this is a homework assignment, I'm not going to solve it here, but I'll give hints. The renormalization of mass is related to the F_1^s Fermi liquid parameter via

$$\frac{m^*}{m} = 1 + \frac{F_1^s}{3} \tag{9.4}$$

Why is this related to F_1^s ? The $l = 1$ Fourier spherical mode of the Fermi surface, shown in Fig. 9.9 corresponds to a simple displacement of the Fermi surface — which is the same as a Galilean boost. One could calculate the energy of this Galilean boost either by starting with the Fermi liquid expression Eq. 9.3, or by realizing that a boost must have energy $N\frac{1}{2}mv^2$, with m the bare mass of the particles! Equating these two gives Eq. 9.4.

---

[9] Recall that for any magnetic system we can write the energy as a function of the magnetization as

$$E(M) = \frac{M^2 \mu_0}{2\chi} - MB + \ldots$$

Figure 9.9: Shifting the Fermi surface is an F_1 deformation. It is also a Galilean boost.

9.5.4 More?

It may seem at this point that we have simply introduced a new fudge factor F for each experiment we want to do. However, once we fix these Fermi liquid parameters, it turns out that many different experiments can be explained. Further almost any experiment we can think of will probe only the first few of the Fermi liquid coefficients.

9.6 Further extensions of Fermi Liquid Theory

9.6.1 Local Dynamical Properties and Boltzmann Transport

Similar to the idea of going from Landau theory of phase transitions to Landau-Ginzburg theory of phase transitions, our next bold step will be to promote the occupations from global to local quantities

$$n_{\mathbf{p},\sigma} \rightarrow n_{\mathbf{p},\sigma}(\mathbf{r})$$

Admittedly this appears to violate the uncertainty relation, since we can't specify **p** and **r** at the same time. However, we can indulge in some amount of semiclassical thinking. As long as we don't try to specify precise values of either, it will still be acceptable. As such, $n(\mathbf{p}, \sigma, \mathbf{r})$ will become some sort of momentum and position phase space density. We can then construct a Boltzmann equation or dynamical theory. We will not derive the Boltzmann equation here, but ...

.. it has solutions that are oscillations of the *shape* of the Fermi surface, without oscillations in the local density. This phenomenon is known as *zero sound*. It was predicted by Landau and then observed in the 1960s in ^{3}He. Note that as the temperature goes to zero, regular sound vanishes. The reason for this is the lack of quasiparticle scattering when the quasiparticles are at low energy. Regular sound is derived by assuming local thermodynamic quantities, such as pressure, which is calculated from a local equation of state (pressure as a function of density). However, if the quasiparticles are not scattering, one never gets thermodynamic equilibrium and resular sound then no longer makes sense.

In contrast, zero sound persists down to zero temeprature, since it is derived without assuming any scattering of quasiparticles (the assumption of Fermi liquid theory!).

9.6.2 Landau-Silin Theory: Long Range Coulomb Interactions

Finally we return to Fermi liquids in metals. These are omnipresent in our world and so are of great interest. The long range Coulomb interaction presents some problems for Fermi liquid theory. However, Landau and Silin (1956) developed a good method to address this, which can be thought of as a combination of Landau theory of Fermi liquids and the RPA or self-consistent Hartree approximation which we apply in two steps:

(1) First, we imagine a Fermi system with short range interaction only. Since the Fock interaction is short range (it requires wavefunction overlap), we can treat this part of the interaction between particles, but we throw out the long range hartree part. With this modified short range interaction, we have something we can treat properly with conventional Fermi liquid theory. We then calculate the properties of this fictitious interaction-truncated Fermi system. For example, we might have

$$\tilde{\chi}^0 = \frac{\partial n}{\partial \mu} = \frac{D^*(E_F)}{1 + F_0^s}$$

(2) Once we have calculated all of these responses, we then add back in the long range Hartree part of the interaction at RPA level. For example,

$$\chi = \frac{\tilde{\chi}^0}{1 - \tilde{V}\tilde{\chi}^0} \tag{9.5}$$

So this approach is just like RPA, except instead of using the noninteracting response χ^0 in Eq. 9.5, we use a response $\tilde{\chi}^0$ which includes Fermi liquid corrections due to the short range part of the interaction. So we see that the compressibility is modified by the mass renormalization and the F_0^s Fermi liquid correction. For example, that in this approach, the Thomas-Fermi wavevector becomes modified to get

$$k_{TF}^2 = \frac{e^2}{\epsilon_0}\frac{D^*(E_F)}{1 + F_0^s} = \frac{e}{\epsilon_0}\tilde{\chi}^0(q = 0, \omega = 0)$$

Chapter 10

Leading up to BCS Theory: Electron Binding

As mentioned way back in chapter 2, the era of superconductivity started in 1911. Yet there was no microscopic understanding of the effect until 1957 when Bardeen[1], Cooper, and Schrieffer (BCS) produced what still remains *the* theory of superconductors.

We already have discussed the general idea that a superconductor can roughly be described as a superfluid (roughly a Bose-Einstein condensate) of charge $2e$ bosons. While this had been discussed prior to BCS, no one took it seriously for the two reasons mentioned at the start of chapter 7: electrons repel and even if you can get electrons to attract each other, in order to get them to bind into a small boson you can treat individually(i.e., binding radius smaller than interboson distance) you need a binding energy on order of the Fermi energy, which is entirely crazy. What will turn out to be crucial is that even a very weak attraction[2] will be sufficient to bind electrons together, at least in a sense. Landau's quip that "you cannot repeal Coulomb's law" was somewhat incorrect[3]. The screening of the Coulomb interaction on very short scales makes the Coulomb repulsion much less effective than you might otherwise fear, and even a weak attraction mechanism can then be important.

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[1] John Bardeen is one of only four people to win two Nobel prizes. In the late 1940's Bardeen was one of the co-inventors of the transistor — the fundamental element of circuitry that powers the information age. However, his boss at Bell labs, William Shockley (who won the prize with Bardeen), was also a pathological personality and made it essentially impossible for Bardeen to continue doing any work on transistors. Bardeen left Bell labs for Urbana where he began work on superconductivity.

[2] Indeed often a weak attraction even in the presence of lots of repulsion!

[3] You might not be able to repeal it, but you can screen it!

10.1 Mechanism of Attraction

First we need to figure out why electrons attract each other. In “conventional” superconductors, the mechanism involves the interaction between the electrons and the vibrations of the crystal lattice – i.e, phonons. This idea was put forth as early as 1950 by people such as Feynman and Frölich.

In more exotic superconductors, including the high T_c perovskite superconductors discovered in the 1980s, the pnictide superconductors discovered in the 2000s' and ^{3}He superfluid (^{3}He pairs at low temperature like a superconductor) it is believed that the mechanism of attraction does not involve phonons. These are much more complicated systems and they remain popular topics of research. In fact, there have been (no exaggeration) over 10^6 publications aimed to understand why the high T_c superconductors superconduct, and still there is no agreement!

For conventional superconductors (which includes the vast majority of supercondutors known), fortunately, there is quite a bit of good evidence that it is the coupling to the phonons that is crucial. A very strong piece of evidence comes from the so-called “isotope effect”. One considers different isotopes of the same material — i.e., adding and subtracting a few neutrons from the nucleus of atoms. The neutrons do nothing to the electronic properties of the material, or the band structure. The only thing they do is to change the frequency of vibration of the atoms by changing their masses. In these conventional superconductors it is usually found that the critical temperature for superconductivity scales as

$$T_c \sim M^{-\alpha} \tag{10.1}$$

where M is the mass of the atomic nucleus, where $\alpha \approx .5$. The fact that the nuclear mass plays any role in the superconductivity is a sure sign that phonons are crucial to the mechanism.

Since this point is fairly important we will give two different calculations which describe how the coupling to phonons generates an attraction between electrons.

10.1.1 Canonical Transformation

Let us write a simple model of electrons and phonons

$$H = H_0 + H_1$$

where H_0 is the Hamiltonian for uncoupled phonons and electrons and H_1 includes the small coupling between the two. We write explicitly

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \hbar\omega \sum_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}}$$

Here the first term is the electrons (and for simplicity of notation, we suppress the spin indices) and the second term is Einstein phonons (with polarization indices suppressed).

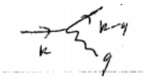

Figure 10.1: Electron-Phonon coupling

The use of Einstein phonons is simply the statement that all of our phonons have the same frequency ω independent of $\mathbf{q}$. We can switch to a real phonon dispersion without too much added complication, but this simplified model will be enough to get the idea.

The coupling between electrons and phonons is given by

$$H_1 = \sum_{\mathbf{q},\mathbf{k}} \left[M\, c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}}\, a^\dagger_{\mathbf{q}} + h.c. \right] = \sum_{\mathbf{q}} \left[M\, \hat{\rho}_{\mathbf{q}}\, a^\dagger_{\mathbf{q}} + h.c. \right] \tag{10.2}$$

where M is an interaction matrix element that usually would be $M_{\mathbf{q}}$ but we will take it as a constant for simplicity. The physics here is that any charge density that builds up is able to couple to phonons[4]. Diagrammatically this coupling is shown in Fig. 10.1

The Hamiltonian $H = H_0 + H_1$ is a complicated interacting Hamiltonian, and is generally difficult to solve. However, we can take advantage of the fact that the coupling constant M is small. This enables us to work perturbatively in this parameter. Our idea is to remove the phonons from consideration and determine what the effective interaction is between electrons. This is known as "integrating out" the phonons[5]. To do this we make a canonical transformation on our Hamiltoninan

$$\mathcal{H} = e^{-S} H e^{S} = H + [H,S] + \frac{1}{2}[[H,S],S] + \ldots$$

The idea is to choose S so that the electron part of the Hamiltonian becomes completely decoupled from the phonons (at the price of introducing an effective interaction between the electrons). We can make this decoupling order by order in the small parameter M, where H_1 is order M and we assume that S is also order M (since if M is zero, we are decoupled with $S = 0$). Let us rewrite the series, order by order in the small parameter

$$\mathcal{H} = \Big(H_0 \Big) + \Big(H_1 + [H_0, S] \Big) + \Big([H_1, S] + \frac{1}{2}[[H_0,S],S] \Big) + \mathcal{O}(small^3)$$

where each set of terms in parenthesis () are of the same order. Let us choose S so as to eliminate the first order term

$$H_1 + [H_0, S] = 0 \tag{10.3}$$

---

[4] There are two main mechanisms by which phonons couple to electrons. The first is piezoelectric coupling whenever a crystal is non-centro-symmetric, where compressing the crystal actually creates an electric field that the electrons then respond to. The second mechanism is so-called deformation potential coupling – where compressing the crystal changes the hopping strength between atomic orbitals and changes the energies of the bands, and hence changes the energies of the electrons.

[5] The nominclature is from path integral language where it really is an integral.

Plugging this back into the expansion we get

$$\mathcal{H} = H_0 + \frac{1}{2}[H_1, S] + \mathcal{O}(small^3)$$

We have thus eliminated the coupling between electrons and phonons at first order, leaving only the second order term, which we call

$$H_{int} = \frac{1}{2}[H_1, S]$$

So that

$$\mathcal{H} = H_0 + H_{int} + \mathcal{O}(small^3)$$

Let us now back up to Eq. 10.3 and try to figure out what operator S satisfies this equation. To determine this, we take the matrix element between two kets

$$\begin{aligned} \langle n|H_1|m\rangle &= -\langle n|[H_0, S]|m\rangle \\ &= -(E_n - E_m)\langle n|S|m\rangle \end{aligned}$$

so

$$\langle n|S|m\rangle = \frac{\langle n|H_1|m\rangle}{E_m - E_n} \tag{10.4}$$

We now want to figure out what H_{int} does to make an effective interaction between electrons. Let us consider two kets $|a\rangle$ and $|b\rangle$ having the same number of phonons excited and we are interested in finding the effective interaction matrix element

$$\langle a|H_{int}|b\rangle$$

This can be evaluated as

$$\begin{aligned} \langle a|H_{int}|b\rangle &= \frac{1}{2}\langle a|[H_1, S]|b\rangle \\ &= \frac{1}{2}\sum_c \left[\langle a|H_1|c\rangle\langle c|S|b\rangle - \langle a|S|c\rangle\langle c|H_1|b\rangle\right] \\ &= \frac{1}{2}\sum_c \langle a|H_1|c\rangle\langle c|H_1|b\rangle \left[\frac{1}{E_b - E_c} + \frac{1}{E_a - E_c}\right] \end{aligned}$$

where in going to the last line we used Eq. 10.4.

Now let us take as given that $|a\rangle$ and $|b\rangle$ both have no excited phonons. Then the state $|c\rangle$ must have one excited phonon, considering the form of the coupling H_1 given in Eq. 10.2. Note that if the intermediate state $|c\rangle$ is of higher energy than either $|a\rangle$ or $|b\rangle$ then the term in the brackets is negative and we have an attractive interaction.

To see this in more detail, consider consider a case where we have for example

$$|b\rangle = c_k^\dagger c_p^\dagger |FS\rangle \tag{10.5}$$

$$|a\rangle = c_{k-q}^\dagger c_{p+q}^\dagger |FS\rangle \tag{10.6}$$

$$|c\rangle = c_{k-q}^\dagger c_p^\dagger a_q^\dagger |FS\rangle \tag{10.7}$$

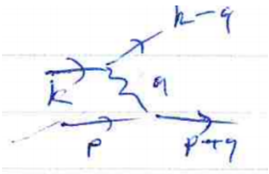

Figure 10.2: Electron-Phonon scattering makes an effective electron-electron interaction.

Thus the process looks like Fig. 10.2 The effective interaction Hamiltonian can then be rewritten as

$$\langle a|H_{int}|b\rangle = \frac{1}{2}\sum_{p,k,q} c^\dagger_{p+q}c_p c^\dagger_{k+q}c_k |M|^2 \left[\frac{1}{\epsilon_k - \epsilon_{k-q} - \hbar\omega} + \frac{1}{\epsilon_{p+q} - \epsilon_p - \hbar\omega}\right]$$

Now if the energy differences between the fermion states are small compared to $\hbar\omega$ then the interaction is attractive. Further if we can drop the energies of the fermions this simplifies even further to the very simple attractive form

$$H_{eff} = -\frac{|M|^2}{\hbar\omega}\sum_q \rho_q\rho_{-q}$$

Fourier transforming, an effective interaction which is constnat in $\mathbf{q}$, one can see that this corresponds to a short ranged attractive interaction between electrons.

10.1.2 RPA Screening and Ion Gas Model

Because the above calculation may seem a bit mysterious, we are going to do a second, almost classical, calculation to show where the attraction comes from. This calculation is based on self-consistent calculations very similar to the RPA that we discussed above in section 8.4.

In this approach we are going to crudely model the background ions as a structureless fluid of moving positive charge. We throw away the lattice and consider the ions as some sort of liquid.

To impliment this approach, let us first remind ourselves of high frequency behavior of charged particles. We derived (in several ways!) in sections 8.3.2 this response given by

$$\delta\rho(\mathbf{q},\omega) = \chi^0(\mathbf{q},\omega)\phi(\mathbf{q},\omega)$$

where here $\delta\rho$ is the induced charge density[6] and

$$\chi^0(\mathbf{q},\omega) = \frac{\mathbf{q}^2\bar{n}e^2}{\omega^2 m} = q^2\epsilon_0\left(\frac{\Omega^2_{e,pl}}{\omega^2}\right)$$

---

[6] Note that above we calculated the induced number density, so this differs by a factor of $-e$.

where $\bar{n}$ is the averege density and $\Omega_{e,pl}$ is the plasma frequency

$$\Omega_{e,pl} = \sqrt{\frac{\bar{n}e^2}{m\epsilon_0}}$$

Recall that this is nothing more than the harmonic oscillations of charged particles in a neutralizing background (See section 8.4.2). For most metals this plasma frequency is very high — up in the several eV range ($>$ 10,000's of K)[7].

We now apply the same idea to the background ions which we view as simply a free fluid of charged particles too — only here the particles have positive charge, and their mass is much much greater than that of an electron. Here the mass is that of the entire positive ion (and recall that a single nucleon is some 1800 times heavier than an electron, and further each ion has many nucleons!). Thus, even for a light metal like aluminum, we have the mass of the nucleon being almost 50,000 times that of the electron. Thus we have a response for the background ion fluid being given by

$$\chi^0_{ion}(\mathbf{q}, \omega) = q^2 \epsilon_0 \left(\frac{\Omega^2_{ion,pl}}{\omega^2} \right)$$

where

$$\Omega_{ion,pl} = \sqrt{\frac{\bar{n}e^2}{M\epsilon_0}} \tag{10.8}$$

with $\bar{n}$ the density of ions e their charge, and M their (very large) mass. This description of the motion of ions as a fluid is a very crude approximation of phonons in a solid. We have

$$\Omega_{ion,pl} \approx \omega_{Debye} \tag{10.9}$$

the characteristic scale of phonons, the which is typically on the order of 100 Kelvin.

At these very low frequencies (compared to the electron plasma frequency) the electron response is approximately the same as if ω were zero. (I.e., ion are extremely slow compared to electrons!). The low frequency response of noninteracting electrons is given by the compressibility

$$\chi^0_e(\omega \approx 0) = -e^2 D(E_F)$$

with $D(E_F)$ being the density of states at the Fermi surface.

Let us now consider an RPA calculation (See section 8.4) of the the response of the coupled system of electrons and ions together. We write the total electrostatic potential as the sum of an external potential and an induced potential

$$\phi^{tot}(\mathbf{q}, \omega) = \phi^{ex}(\mathbf{q}, \omega) + \phi^{ind}(\mathbf{q}, \omega)$$

---

[7] To see this, consider a case where the density is $1/a_0^2$ with a_0 the Bohr radius. In this case it is easy to see that the plasma frequency is essentially the Rydberg.

where the induced potential is due to the Coulomb potential from both the electrons and the ions, which in turn is created by their own response to the total electrostatic potential

$$\begin{aligned}\phi^{tot}(\mathbf{q},\omega) &= \phi^{ex}(\mathbf{q},\omega) + \tilde{V}(\mathbf{q})\left[\delta\rho^{e}(\mathbf{q},\omega) + \delta\rho^{ion}(\mathbf{q},\omega)\right] \\ &= \phi^{ex}(\mathbf{q},\omega) + \tilde{V}(\mathbf{q})\left[\chi^0_e\phi^{tot}(\mathbf{q},\omega) + \chi^0_{ion}(\mathbf{q},\omega)\phi^{tot}(\mathbf{q},\omega)\right]\end{aligned}$$

Solving, we obtain

$$\phi^{tot}(\mathbf{q},\omega) = \frac{\phi^{ext}(\mathbf{q},\omega)}{1 - \tilde{V}(\mathbf{q})\left[\chi^0_e + \chi^0_{ion}(\mathbf{q},\omega)\right]}$$

which gives the general screening of an externally applied potential. Similarly any potential between any two charged particles will be screened, and we have an effective interaction

$$\begin{aligned}V^{eff}(\mathbf{q},\omega) &= \frac{\tilde{V}(\mathbf{q})}{1 - \tilde{V}(q)\left[\chi^0_e + \chi^0_{ion}(\mathbf{q},\omega)\right]} \\ &= \frac{\tilde{V}(\mathbf{q})}{1 + \frac{k^2_{TF}}{q^2} - \frac{\Omega^2_{ion,pl}}{\omega^2}}\end{aligned}$$

where k_{TF} is the Thomas-Fermi screening wavevector of section 8.1.

There are several key points to note about this result.

- Without phonons this just recovers regular Thomas-Fermi screening. (We can Fourier transform to obtain the same Yukawa interaction as in Eq. 8.5 and 8.30).
- For high frequency $\omega \gg \Omega_{ion,pl} \approx \omega_{Debye}$ the ion term vanishes and the phonons don't matter.
- In the limit of $\omega \to 0$ we obtain perfect screening as the ions fluid can always perfectly screen a fully static potential (the denominator explodes and gives a zero result).
- Crucially, for small ω the ion term in the denominator dominates and we get an *attractive* interaction![8]

The physical picture we should have here is that when an electron moves through the ions, it polarizes the ions, but the ions move slowly. The ions respond and build up a screening charge that is maintained for a long time after the electron is gone. Another electron can be attracted to this region for some time after the electron is gone. This constitutes the low frequency attractive interaction between electrons.

---

[8] It turns out that this oversimplified model where we treat the ions as being a fluid and perform RPA-like calculations greatly *over*-estimates the strength of the resulting attractive interaction. Nonetheless, it gives an idea of where the attraction comes from.

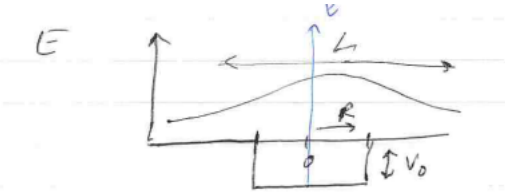

Figure 10.3: A square well potential extending to distance R and a wavefunction extended to a distance L.

10.2 Bound States and the Cooper Problem

10.2.1 Non-Existence of Weakly Bound States in 3D

We have thus developed a way to justify that a (weak) attractive interaction may be developed between electrons. We can now ask a fundamental question:

Question:

Given a very weak attractive potential in D dimensions, does there exist a bound state

Answers:

In $D < 2$ the answer is yes.
In $D > 2$ the answer is no.
$D = 2$ is complicated, but the answer is usually yes.

Since the result of this statement is important and (except for $D = 2$) the result is easy to prove, it is worth actually proving it. (In fact our proof will not be fully rigorous, but it will give the right ideas).

Note that since we are thinking about superconductivity we are really concerned with forming a bound state between two particles, but we can go to relative coordinates with a reduced mass and think about this as forming a bound state of a single particle in a potential.

Let us consider a potential in general dimension D although we will draw the potential in 1d for obvious reasons as shown in Fig. 10.3. The detailed shape of the potential doesn't matter much, so we will choose it to be a square well which extends to some radius R. What is crucial is that at infinite distance from the origin, the potential must go strictly to zero.

If the potential is infinitessimly small (but attractive), we would like to know whether there a bound state. In other words, is there an eigenstate with energy below zero? If so, then by WKB approximation we can show that the state is bound near position zero and the wavefunction must decay as $e^{-|x|/L}$ with L very long if the bound state is very close to zero energy.

If the eigenstate is very weakly bound, we must assume that the binding radius L

is large. However, we must also have normalization

$$\int d^D r \; |\psi|^2 = 1$$

so that we must assume the wavefunction magnitude is roughly

$$|\psi| \sim L^{-D/2}$$

Now let us try to estimate the potential and kinetic energy of the system. With the box-like potential in D dimensions we simply want the integral of the squared wavefunction times the potential inside the box

$$\text{Potential Energy} = -V_0 \int_{|\mathbf{r}|<R} d_r^D \; |\psi|^2 \sim -V_0 (R/L)^D$$

On the other hand, the kinetic energy should be

$$\text{Kinetic Energy} = \frac{\hbar^2}{2mL^2}$$

Thus the total energy is

$$\text{KE+PE} = \frac{\hbar^2}{2mL^2} - V_0 \left(\frac{R}{L}\right)^D$$

For $D < 2$ this always becomes negative for large enough L, for arbitrarily small V_0. Thus there is always a bound state in $D < 2$. For $D > 2$ there is generally no bound state for very small V_0 (although a stronger V_0 can certainly form a bound state). Since we are mainly concerned with three dimensional materials this seems like a rather discouraging result — no bound states will form if an attraction is weak[9].

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10.2.2 The Cooper Problem: Bound States in The Presence of a Fermi Sea

The crucial discovery by Leon Cooper (1956) is that the presence of a Fermi sea completely changes the situation. We will see that in *any* dimension, in the presence of a Fermi sea an *arbitrarily* weak attractive potential will form a bound state! The key here is that the Pauli exclusion principle facilitates electron binding. Let us see how this works.

Suppose we start with a Fermi sea and we add two electrons. These two electrons can only be added above the Fermi wavevector k_F.

Let us write an appropriate trial bound state for the two added electrons

$$\psi(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) = \chi(\sigma_1, \sigma_2)\phi(\mathbf{r}_1, \mathbf{r}_2) \tag{10.10}$$

---

[9] Clearly the $D = 2$ case will be complicated since the kinetic and potential energies scale the same way.

where, as usual, we have now separated the spatial and spin part of the wavefunction. We can choose to have the electrons in either a spin singlet or a spin triplet – either is possible, and in fact the argument doesn't change much. Since electron pairing in most superconductors have the spins in singlet pairs, we will choose this case to study. So we write[10] the singlet form for the spin wavefunction

$$|\chi\rangle = \frac{1}{\sqrt{2}}(\,|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle\,) \tag{10.11}$$

Since the spin part of the wavefunction is antisymmetric we must have the spatial part of the wavefunction be symmetric, so we propose the following:

$$\phi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{V}\sum_{|\mathbf{k}|>k_F} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} g_{\mathbf{k}} \tag{10.12}$$

where we have added a factor of the volume of the system V for convenient normalization. In order to have the wavefunction be symmetric between $\mathbf{r}_1$ and $\mathbf{r}_2$ we have to choose $g_{\mathbf{k}} = g_{-\mathbf{k}}$. In fact for simplicity, if we are considering a rotationally invariant system we can choose $g_{\mathbf{k}}$ to be a function of $|\mathbf{k}|$ only so we write $g_{|\mathbf{k}|}$ or sometimes g_k..

There are several key things to note about this trial wavefunction.

- Note that in the sum over wavevectors we have only included wavevectors $k > k_F$. This is because we are assuming there is already a Fermi sea and all states below k_F are already filled.
- The trial wavefunction has no dependence on $\mathbf{r}_1+\mathbf{r}_2$. This means that we are putting the center of mass of the pair into a $\mathbf{K} = 0$ momentum state. This is equivalent to saying that we always occupy $\mathbf{k}$ with $-\mathbf{k}$ at the same time in a pair.
- It is perhaps simpler to write the wavefunction 10.10-10.12 in second quantized form where we have
$$|\Psi\rangle = \frac{1}{V}\sum_{|\mathbf{k}|>k_F} g_{\mathbf{k}}\; c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k},\downarrow}|FS\rangle$$
where $|FS\rangle$ is the filled Fermi sea. The anti-commutations of the creation operator ensure we obtain a singlet state.

Let us now assume there is a weak attractive interaction $U(\mathbf{r}_1 - \mathbf{r}_2)$ between the two added electrons. Let us try to solve the Schroedinger equation for the two electrons to see if we find a bound state. We have the Schroedinger equaiton (in shorthand form)

$$\left(\hat{\mathrm{KE}} + \hat{\mathrm{PE}} - E\right)|\psi\rangle = 0$$

Letting $\epsilon_{\mathbf{k}}$ be the kinetic energy of an electron with wavevector $\mathbf{k}$. We then have

$$\sum_{|\mathbf{k}|>k_F} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} g_{\mathbf{k}}\left[2\epsilon_{\mathbf{k}} + U(\mathbf{r}_1 - \mathbf{r}_2) - E\right] = 0$$

---

[10] In another language the singlet is $\chi(\uparrow,\downarrow) = -\chi(\downarrow,\uparrow) = 1/\sqrt{2}$ and $\chi(\uparrow,\uparrow) = \chi(\downarrow,\downarrow) = 0$.

To solve this, we Fourier transform applying

$$\int d^D(\mathbf{r_1} - \mathbf{r}_2)\ \ e^{-i\mathbf{q}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}$$

where we define the Fourier tranformed potential via

$$U(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{q}} \tilde{U}_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}$$

The Schroedinger equation becomes

$$(2\epsilon_{\mathbf{q}} - E)\, g_{\mathbf{q}} + \frac{1}{V}\sum_{|\mathbf{k}|>k_F} \tilde{U}_{\mathbf{q}-\mathbf{k}}\ g_{\mathbf{k}} = 0 \tag{10.13}$$

This is still a rather difficult equation to solve. The trick here is to choose a particularly simple interaction U that roughly represents the type of interaction we might actually have in a real system, but is still simple enough to work with. We recall that when we derived a phonon-mediated attraction, it was attractive for low frequencies only. We thus propose the following very simplified interaction

$$\tilde{U}_{\mathbf{q},\mathbf{k}} = \begin{cases} -U_0 & \text{if } \epsilon_{\mathbf{k}} \text{ and } \epsilon_{\mathbf{q}} \text{ are both} \\ & \text{within } \hbar\omega_{Debye} \text{ of the Fermi surface} \\ & \\ 0 & \text{otherwise} \end{cases}$$

Note that this is a bit of a strange interaction. We write this as a function of two wavevectors $\mathbf{k}$ and $\mathbf{q}$ which are the Fourier transforms of $\mathbf{r}_1$ and $\mathbf{r}_2$. However, the resulting interaction is not a function of $\mathbf{k} - \mathbf{q}$ only, meaning that in real space this is not actually translationally invariant! Nonetheless, this interaction has nice analytic properties, so we will use it.

Replacing $\tilde{U}_{\mathbf{q}-\mathbf{k}}$ with $\tilde{U}_{\mathbf{q},\mathbf{k}}$ in Eq. 10.13 we obtain

$$(2\epsilon_{\mathbf{q}} - E)\, g_{\mathbf{q}} - \frac{U_0}{V}\sum_{\substack{|\mathbf{k}|>k_F \\ \epsilon_{\mathbf{k}}<E_F+\hbar\omega_{Debye}}} g_{\mathbf{k}} = 0 \tag{10.14}$$

which is now simple enough to solve.

Next we use the fact that we wanted to take $g_{\mathbf{k}}$ to be a function of $|\mathbf{k}|$ only, and further for a rotationally invariant system, we can say that k is a function of the kinetic energy ϵ. (Usually we write it the other way, $\epsilon(k)$ but here we will write $k(\epsilon)$). We can then replace the second term in Eq. 10.14 with

$$\frac{U_0}{V}\sum_{\substack{|\mathbf{k}|>k_F \\ \epsilon_{\mathbf{k}}<E_F+\hbar\omega_{Debye}}} g_{\mathbf{k}} = U_0 D(E_F)\int_{E_F}^{E_F+\hbar\omega_{Debye}} d\epsilon'\, g_{k(\epsilon')} \equiv C \tag{10.15}$$

where $D(E_F)$ is the density of states per unit volume at the Fermi surface (which we will assume is just a constant over the small energy range of interest). We have defined the value of this integral to be called C.

We can then invert Eq. 10.14 to give

$$\begin{aligned} g_{k(\epsilon)} &= \frac{U_0 D(E_F) \int_{E_F}^{E_F+\hbar\omega_{Debye}} d\epsilon' \, g_{k(\epsilon')}}{2\epsilon - E} \\ &= \frac{C}{2\epsilon - E} \end{aligned}$$

We can then multiply both sides of this equation by $U_0 D(E_F)$ and integrate both sides of this equation as in Eq. 10.15 in order to obtain C on the left

$$C = U_0 D(E_F) \int_{E_F}^{E_F+\hbar\omega_{Debye}} d\epsilon' \frac{C}{2\epsilon' - E}$$

Cancelling C we then obtain

$$\frac{1}{D(E_F)U_0} = \int_{E_F}^{E_F+\hbar\omega_{Debye}} d\epsilon' \frac{1}{2\epsilon' - E} = \frac{1}{2} \ln \left[\frac{2(E_F + \hbar\omega_{Debye}) - E}{2E_F - E} \right]$$

which can then be exponentiated to give

$$\exp\left(\frac{2}{U_0 D(E_F)}\right) = 1 + \frac{2\hbar\omega_{Debye}}{2E_F - E} \tag{10.16}$$

Now for small U_0, the left is very large, which means that the right needs to be large too, meaning that $2E_F - E$ is very small but positive. This means that there is an eigenstate with energy $E < 2E_F$. This must be a bound state!! (Since the energy of two noninteracting electrons above the Fermi sea can be no lower than $2E_F$.)

We can simplify a bit more here. For small U_0 both left and right of Eq. 10.16 are large, which means we can drop the 1 on the right hand side. Thud giving

$$\exp\left(\frac{2}{U_0 D(E_F)}\right) = \frac{2\hbar\omega_{Debye}}{2E_F - E} \tag{10.17}$$

or equivalently the binding energy is given by

$$\text{Binding Energy} = 2E_F - E = 2\,\hbar\omega_{Debye} \exp\left(\frac{-2}{U_0 D(E_F)}\right) \tag{10.18}$$

There are two crucial things to point out about this result:

First, without the Fermi sea, there is no bound state. To see this, let the density of states at the Fermi surface $D(E_F)$ go to zero (as it does in 3d as the Fermi sea gets smaller and smaller). Then the binding energy goes to zero.

Second: Note that the expression for the binding energy is *non-analytic* in the potential strength U_0. No order in perturbation theory would ever find this result. To see this consider expanding a function like $e^{-1/x}$ around $x = 0$ in a taylor series. *All* derivatives at $x = 0$ vanish — so this function, while smooth, has zero radius of convergence around $x = 0$. So too does the expression for the binding energy if we try to expand it for small U_0. This nonanalyticity is one reason why discovering the binding of electrons on top of a Fermi sea was so difficult!

Chapter 11

BCS Theory

Given that two electrons just above the Fermi surface form a bound state even for weakly attractive interactions, we can see that the whole Fermi surface must become unstable: First two electrons jump above the Fermi sea to form a bound state and lower their energies, then two more, and so forth, until all of the electrons near the Fermi surface are paired up. The question is how do we describe such a state of matter now?

In 1956, many of the top physics minds in the world, both in the West and in the Soviet Union, were working on superconductivity – people like Feynman and Landau[1]. After seeing Cooper's calculation of the binding of electrons above a Fermi sea, the world was hot on the chase to figure out *the* theory of superconductivity. Bardeen had hired Cooper to come to Urbana and work with him. Unfortunately (or perhaps fortunately) in the fall of 1956, Bardeen won the Nobel prize[2] for the invention of the transisitor, and he had to pause his research to go to Sweden to collect his prize[3]. While he was gone, his graduate student, Robert Schrieffer, was left to puzzle over the problem with Cooper. The two of them went to some conferences in New York City, and while Schrieffer was on the subway he cracked the problem. Within a few months they had essentially worked out most of the details of the modern theory of superconductivity[4]. The general idea is to make something that looks a bit like a BEC of pairs of electrons. We will see that the trial wavefunction has some properties that makes it look like a BEC and some properties

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[1] This was an era when many top scientists thought there was not much interesting in high energy physics for a while.

[2] Along with William Shockley and Walter Brattain

[3] Bardeen only brought one of his three children with him to Stockholm for the prize ceremony since the other two were studying at Harvard and he didn't want to interrupt their studies (Although he was very happy to win the prize he fundamentally did not think prizes should be that important!). King Gustav chided him for not bringing all his children, and Bardeen promised that he would bring the whole family for his next Nobel prize. Sixteen years later he kept that promise.

[4] Schrieffer's PhD thesis is one of the most beautiful pieces of PhD research one could possibly imagine. It is essentially identical to his later book on superconductivity which is considered a classic of the field. Like many geniuses Schrieffer struggled with his mental health. Much later in life Schrieffer was sentenced to two years in prison for vehicular manslaughter having killed two people in a crash while he was driving with a suspended license.

that make it distinct from a BEC.

11.1 The BCS wavefunction

11.1.1 Fixed N wavefunction

Recall how we construct a BEC from bosons. We can write a creation operator for bosons in some orbital χ

$$a_\chi^\dagger = \int \mathbf{dr}\ \chi(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})$$

Then a BEC with N particles can be written as

$$|\psi_N^{BEC}\rangle = (a_\chi^\dagger)^N|0\rangle$$

Can we do something similar with fermion pairs? Let us define a pair creation operator (assuming the pair is a singlet)

$$\begin{aligned}\tilde{a}^\dagger &= \int \mathbf{dr}_1 \int \mathbf{dr}_2\ g(\mathbf{r}_1-\mathbf{r}_2)\ \hat{\psi}_\uparrow^\dagger(\mathbf{r}_1)\psi_\downarrow^\dagger(\mathbf{r}_2) \\ &= \sum_{\mathbf{k}} g_{\mathbf{k}}\ c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger\end{aligned}$$

which creates a pair of electrons in the orbital

$$g(\mathbf{r}_1,\sigma_1;\mathbf{r}_2,\sigma_2) = \frac{1}{\sqrt{2}}(\,|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle\,)g(\mathbf{r}_1-\mathbf{r}_2)$$

In the simple case where the orbital $g(\mathbf{r})$ is radially symmetric, we can take $g_{\mathbf{k}}$ to be a real function of $|\mathbf{k}|$ only which we might write as g_k.

It is sometimes useful to define a pair creation operator for creating singlet pairs in opposite momentum eigenstates.

$$P_{\mathbf{k}}^\dagger = c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger \tag{11.1}$$

such that the creation operator for a pair in orbital $g(\mathbf{r}_1-\mathbf{r}_2)$ can be written as

$$\tilde{a}^\dagger = \sum_{\mathbf{k}} g_{\mathbf{k}}\ P_{\mathbf{k}}^\dagger$$

We might wonder if the operator $\tilde{a}^\dagger$ and $\tilde{a}$ are proper canonical boson creation and annihilation operators. For this we would like to have

$$[\tilde{a},\tilde{a}^\dagger] = 1$$

or, indeed, any constant on the right hand side would work since we could rescale the operators to make it into unity. However, direct calculation instead gives us

$$\begin{aligned}[\tilde{a},\tilde{a}^\dagger] &= \sum_{\mathbf{k},\mathbf{k}'} g^*_{\mathbf{k}'} g_{\mathbf{k}} \left[c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow}, c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow}\right] \\ &= \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \left(1 - n_{\mathbf{k},\uparrow} - n_{\mathbf{k},\downarrow}\right)\end{aligned}$$

So we see that these operators are not quite bosons. However, for most **k**'s not near the Fermi surface the operators $n_{\mathbf{k}}$ on the right hand side are going to be fixed anyway (far below the Fermi surface they will be filled, far above they will be empty) so we can think of the right hand side as being "mostly" a constant, and see how far we get with these "pseudo"-bosons.

Let us now consider trying to make a BEC-like wavefunction out of these operators. We try to multiply occupy this orbital by writing

$$|\psi_N^{BCS}\rangle = (\tilde{a}^\dagger)^N|0\rangle$$

This wavefunction can be explicitly evaluated to give the following result

$$\psi_N^{BCS} = \mathrm{Pf}(g) \equiv \mathcal{A}\left[g(1,2)g(3,4)g(5,6)\ldots g(2N-1,2N)\right] \tag{11.2}$$

here Pf stands for "Pfaffian"[5] which is a mathematical shorthand for what is written on the far write. We have used the notation $g(1,2)$ to mean $g(\mathbf{r_1},\sigma_\mathbf{1};\mathbf{r_2},\sigma_\mathbf{2})$ and $\mathcal{A}$ means we should antisymmetrize over all possible pairings of electrons with each other. For example

$$\mathcal{A}\left[g(1,2)g(3,4)\right] = g(1,2)g(3,4) - g(1,3)g(2,4) + g(1,4)g(2,3)$$

This expression Eq. 11.2 is the fixed N version of the BCS wavefunction. While it is nice to write it out, and see how this wavefunction generates a sum of all possible pairings of electrons with each other, this particular form of the wavefunction is close to useless for doing any calculations!

11.1.2 Coherent State Wavefunction

Recall we can write a coherent state expression for a BEC

$$|\psi_{BEC}\rangle = e^{\alpha a^\dagger}|0\rangle$$

So let us try something similar for our paired fermions

$$\begin{aligned}|\psi_{BCS}\rangle &= e^{\alpha\tilde{a}^\dagger}|0\rangle \\ &= e^{\alpha\sum_{\mathbf{k}} g_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow}}|0\rangle \\ &= \left[\prod_{\mathbf{k}} e^{\alpha g_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow}}\right]|0\rangle\end{aligned}$$

---

[5] Named for Johann Friedrich Pfaff, 1765-1825.

However here we note that since the pairs are made up of fermions we cannot create two of them in the same **k** states, i.e.,

$$\left(c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right)^2 = 0$$

So when we expand the exponential we have

$$e^{\alpha g_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}} = 1 + \alpha g_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}$$

with no quadratic or higher order term. Thus our wavefunction can be written as

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} \left(1 + \alpha g_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right)|0\rangle \tag{11.3}$$

As in the case of the coherent state BEC, this wavefuntion has an indefinite number of particles. Furthermore, it is not properly normalized, that is

$$\langle\psi_{BCS}|\psi_{BCS}\rangle \neq 1$$

So our first task will be to calculate the normalization so that we can fix this problem.

$$\langle\psi_{BCS}|\psi_{BCS}\rangle = \langle 0|\prod_{\mathbf{k}'}\left(1 + \alpha^* g^*_{\mathbf{k}'}\, c_{-\mathbf{k}',\downarrow}c_{\mathbf{k}',\uparrow}\right)\prod_{\mathbf{k}}\left(1 + \alpha g_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right)|0\rangle$$

We can simplify this calculation by considering each **k** orbital separately where $|0_{\mathbf{k}}\rangle$ means the vacuum for that orbital (i.e., the unfilled orbital for both $\mathbf{k},\uparrow$ and $-\mathbf{k},\downarrow$). We thus have

$$\begin{aligned}\langle\psi_{BCS}|\psi_{BCS}\rangle &= \prod_{\mathbf{k}}\langle 0_{\mathbf{k}}|\left(1 + \alpha^* g^*_{\mathbf{k}}\, c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}\right)\left(1 + \alpha g_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right)|0_{\mathbf{k}}\rangle \\ &= \prod_{\mathbf{k}}\left(1 + |\alpha g_{\mathbf{k}}|^2\right) \qquad (11.4)\end{aligned}$$

This non-standard normalization is inconvenient so we make the following definitions

$$u_{\mathbf{k}} = \frac{1}{\sqrt{1 + |\alpha g_{\mathbf{k}}|^2}} \tag{11.5}$$

$$v_{\mathbf{k}} = \frac{\alpha g_{\mathbf{k}}}{\sqrt{1 + |\alpha g_{\mathbf{k}}|^2}} \tag{11.6}$$

such that

$$\alpha g_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}} \tag{11.7}$$

and we have the normalization condition

$$|u_{\mathbf{k}|}|^2 + |v_{\mathbf{k}}|^2 = 1 \tag{11.8}$$

If we now take our BCS wavefunction, Eq. 11.3 and divide through by the square root of the normalization constant Eq. 11.4 we obtain the normalized form of the BCS wavefunction

$$|\psi_{BCS}^{normalized}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) \tag{11.9}$$

which properly satisfies

$$\langle \psi_{BCS}^{normalized} | \psi_{BCS}^{normalized} \rangle = 1$$

This is the form of the BCS wavefunction which is most commonly used. As such we will drop the superscript ^{normalized} henceforth.

At this point we have a form for a trial wavefunction, but we still don't know what to use as the parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, or equivalently we don't know $\alpha g_{\mathbf{k}}$, or equivalently we don't know the shape of the orbital $g(\mathbf{r})$ of the bound state of two electrons. To find this we must choose a Hamiltonian and our plan will be to treat the shape of the orbital $g(\mathbf{r})$ (or equivalently $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$) as a variational parameter, and we will minimize the energy of the Hamiltonian with respect to variations in this quantity.

11.2 BCS Hamiltonian, Energy Minimization, and Gap Equation

The type of Hamiltonian for interacting electrons that we have been working with so far has been roughly of the form

$$H = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma} \, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\substack{\mathbf{k_1},\mathbf{k_2},\mathbf{k_3},\mathbf{k_4} \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} v_{\substack{\mathbf{k_1},\mathbf{k_2},\mathbf{k_3},\mathbf{k_4} \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} \;\; c^\dagger_{\mathbf{k_1},\sigma_1} c^\dagger_{\mathbf{k_2},\sigma_2} c_{\mathbf{k_4},\sigma_4} c_{\mathbf{k_3},\sigma_3}$$

where we have made the conventional substitution

$$\xi_{\mathbf{k},\sigma} = \epsilon_{\mathbf{k},\sigma} - \mu$$

which is just the energy measured from the Fermi surface[6].

While even this is an approximation (our interaction, recall, actually is frequency dependent strictly speaking!), it is still too complicated to work with.

Instead let us follow the ideas of Cooper and grossly simplify the Hamiltonian, So let us write the very approximate interaction

$$H_{BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma} \, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \;\; c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} \tag{11.10}$$

---

[6] Strictly speaking here our Hamiltonian with this shift of μ is actually giving us $E - \mu N$. It is quite crucial to keep track of the chemical potential here since our system has an indefinite particle number and we must count a free energy μ each time a particle enters the system.

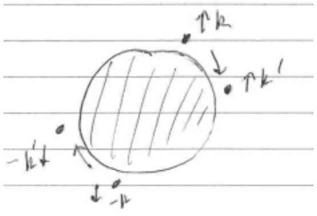

Figure 11.1: this is the caption

where we assume $V_{\mathbf{k},\mathbf{k}'} = V_{\mathbf{k}',\mathbf{k}}$ so that the Hamiltonian is hermitian. For simplicity we will usually assume V is real and attractive (although this is not entirely necessary).

Let us examine this Hamiltonian in a bit of depth. First of all, it is conceptually useful to use the pair creation operator from Eq. 11.1. The BCS Hamiltonian can then be rewritten more succinctly as

$$H_{BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\; P^\dagger_{\mathbf{k}} P_{\mathbf{k}'} \tag{11.11}$$

This simply scatters a pair of electrons $(\mathbf{k}', \uparrow; -\mathbf{k}', \downarrow)$ to new momenta $(\mathbf{k}, \uparrow; -\mathbf{k}, \downarrow)$ with the assumption that both $\mathbf{k}$ and $\mathbf{k}'$ are sufficiently close to the Fermi surface. This process is schematically shown in Fig. 11.1.

The interaction term of the BCS Hamiltonian may seem like it is a tremendously crude simplifiction. However, it turns out to give the right physics of superconductivity so we will use it.[7]

So now our plan is to calculate the energy of the BCS Hamiltonian

$$E = \langle \psi_{BCS} | H_{BCS} | \psi_{BCS} \rangle \tag{11.12}$$

and then minimize over the variational parameters $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ subject to the normalization constraint Eq. 11.8.

To evaluate the expectation of the energy we will need to evaluate a number of simple expectations, like

$$\begin{aligned} \langle \psi_{BCS} | c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} | \psi_{BCS} \rangle &= \langle 0_{\mathbf{k}} | \left(u^*_{\mathbf{k}} + v^*_{\mathbf{k}} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow;} \right) | c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} | \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) | 0_{\mathbf{k}} \rangle \\ &= |v_{\mathbf{k}}|^2 \end{aligned}$$

and similarly for the occupation of down spin electrons. We will also want to know

$$\begin{aligned} \langle \psi_{BCS} | c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} | \psi_{BCS} \rangle &= \langle 0_{\mathbf{k}} | \left(u^*_{\mathbf{k}} + v^*_{\mathbf{k}} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow;} \right) | c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} | \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) | 0_{\mathbf{k}} \rangle \\ &= v^*_{\mathbf{k}} u_{\mathbf{k}} \end{aligned} \tag{11.13}$$

---

[7] Many years after BCS theory was first developed, renormalization group calculations were used to show that the only "relevant" terms in any interaction close to a Fermi surface are precisely those that are kept in the BCS Hamiltonian.

and similarly

$$\langle\psi_{BCS}|c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}|\psi_{BCS}\rangle = u_k^* v_k \tag{11.14}$$

Using these relations we evaluate Eq. 11.12 with the Hamiltonian 11.10 to obtain

$$E = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}}|v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}^* u_{\mathbf{k}} u_{\mathbf{k}'}^* v_{\mathbf{k}'}$$

where the factor of 2 in front of the first term is the sum over two spin states.

Now recalling that we are interested in a pairing wavefunction $g(\mathbf{r}_1 - \mathbf{r}_2)$ which is symmetric, this means we can take $g(\mathbf{r}) = g(-\mathbf{r})$ and hence $g_{\mathbf{k}}$ real. This further means we can take $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ both real. With the constraint 11.8 it is then convenient to simply define

$$\begin{aligned} v_{\mathbf{k}} &= \cos\theta_{\mathbf{k}} && (11.15)\\ u_{\mathbf{k}} &= \sin\theta_{\mathbf{k}} && (11.16)\end{aligned}$$

in which case the variational energy is given by

$$E = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}} \cos^2\theta_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, \sin\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}}\sin\theta_{\mathbf{k}'}\cos\theta_{\mathbf{k}'}$$

We now use some convenient trig identities $\cos^2\theta = (1+\cos 2\theta)/2$ and $\sin\theta\cos\theta = (\sin 2\theta)/2$ to rewrite the energy as

$$E = \sum_{\mathbf{k}} \xi_{\mathbf{k}}(1+\cos 2\theta_{\mathbf{k}}) + \frac{1}{4}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}'}$$

We minimize this energy with respect to the parameters $\theta_{\mathbf{q}}$ by setting $\partial E/\partial\theta_{\mathbf{q}} = 0$ to obtain

$$0 = -2\xi_{\mathbf{q}}\sin 2\theta_{\mathbf{q}} + \cos 2\theta_{\mathbf{q}} \sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \sin 2\theta_{\mathbf{k}} \tag{11.17}$$

where the second term is twice as big as one might expect because we differentiate both sign terms and we have used the expected symmetry $V_{\mathbf{k},\mathbf{k}'} = V_{\mathbf{k}',\mathbf{k}}$.

It is now convenient to define the following object known as the "BCS gap function" (for reasons we will discover soon this will be closely related the superconducting energy gap for low energy excitations):

$$\Delta_{\mathbf{q}} = -\frac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \sin 2\theta_{\mathbf{k}} \tag{11.18}$$

I realize we are in the midst of doing a lot of algebra, but this object is of great physical significance. In order to better understand it, let us unpack the definition — recalling that

$\sin 2\theta = 2\sin\theta\cos\theta$ we have

$$\begin{aligned}\Delta_{\mathbf{q}} &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \sin\theta_{\mathbf{k}} \cos\theta \\ &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}}\, u^*_{\mathbf{k}} v_{\mathbf{k}} \end{aligned} \tag{11.19}$$

Even though we had assumed above that u and v were real, we write them here as generally complex. The reason for this is that in the more general case where we consider more complicated pairing with complex u and v, we will still want to use Eq. 11.19 to define $\Delta_{\mathbf{q}}$. Unpacking this one step further by using Eq. 11.14 we obtain the more physical definition of the gap function in terms of the so-called "anomalous correlator"[8]

$$\Delta_{\mathbf{q}} = -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}\rangle \tag{11.20}$$

Returning now to Eq. 11.17 and substituting in the gap function we obtain

$$\tan 2\theta_{\mathbf{q}} = \frac{1}{\xi_{\mathbf{q}}}\frac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \sin 2\theta_{\mathbf{k}} = \frac{-\Delta_{\mathbf{q}}}{\xi_{\mathbf{q}}} \tag{11.21}$$

From this expression we hope to determine $\sin\theta$ and $\cos\theta$ (and hence u and v and hence the actual wavefunction!). To do this we need a bit more trigonometry. Using $1+\tan^2\theta = \sec^2\theta$ gives us

$$\cos 2\theta_{\mathbf{q}} = \frac{\pm 1}{\sqrt{1+\tan^2 2\theta_{\mathbf{q}}}} = \frac{-\xi_{\mathbf{q}}}{\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2}} \tag{11.22}$$

$$\sin 2\theta_{\mathbf{q}} = \frac{\pm \tan 2\theta_{\mathbf{q}}}{\sqrt{1+\tan^2 2\theta_{\mathbf{q}}}} = \frac{\Delta_{\mathbf{q}}}{\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2}} \tag{11.23}$$

The unknown signs are assigned on the far right so that Eq. 11.21 comes out correctly (We could alternately multiply both terms by -1 and everything would still work). Also note that we have used $|\Delta_{\mathbf{q}}|$ in the denominator here which turns out to be the correct expression when the quantity is complex.

Since we have now obtained $\sin 2\theta$ we can plug Eq. 11.23 into Eq. 11.18 to obtain

$$\Delta_{\mathbf{q}} = -\frac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{\sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}} \tag{11.24}$$

This important equation is known as the "BCS gap equation" and it holds extremely generally for any singlet superconductor.

---

[8] As in the case of using $\langle\psi^\dagger\rangle$ as an order parameter for a Bose condensate, we have chosen an order parameter which involves having an indefinite number of particles in the system, and is strictly zero if the number of particles is fixed. As in the Bose case with greater work it is possible to formulate superconductivity for systems of fixed particle number, although it is substantially more complicated.

At this point, although the gap equation is in principle solvable for any $V_{\mathbf{q},\mathbf{k}}$ it is only analytically solvable for extremely simple forms — we will choose one such form. Recall that we expect the interaction to be attractive only if the energy of the electron is within $\hbar\omega_{Debye}$ of the Fermi surface. Thus a very crude representaion of this physics would be

$$V_{\mathbf{q},\mathbf{k}} = \left\{ \begin{array}{lll} -V_0 & \text{if} & |\xi_{\mathbf{k}}|, |\xi_{\mathbf{q}}| < \hbar\omega_{Debye} \\ 0 & \text{otherwise} & \end{array} \right. \tag{11.25}$$

with V_0 positive corresponding to an attractive interaction. We then claim that with this form of V, the gap equation is solved by the gap function

$$\Delta_{\mathbf{q}} = \left\{ \begin{array}{lll} \Delta & \text{if} & |\xi_{\mathbf{q}}| < \hbar\omega_{Debye} \\ 0 & \text{otherwise} & \end{array} \right. \tag{11.26}$$

Plugging in this this form of the interaction (Eq. 11.25) and gap function (Eq. 11.26) into the gap equation (Eq. 11.24), cancelling Δ on both sides, we obtain a solution for the scalar gap function Δ given by the solution of the equation (with Δ assumed real here)

$$1 = \frac{V_0}{2} \sum_{\substack{\mathbf{k} \\ \xi_{\mathbf{k}} < \hbar\omega_{Debye}}} \frac{1}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} \tag{11.27}$$

We will see below that Δ will represent the energy range around the Fermi surface where there are no excitations — i.e., a gap (hence the name).

This equation can now be simplified a bit further by replacing the sum over $\mathbf{k}$ with an integral with a density of states

$$\sum_{\substack{\mathbf{k} \\ \xi_{\mathbf{k}} < \hbar\omega_{Debye}}} \rightarrow \frac{1}{2} \int_{\mu-\hbar\omega_{Debye}}^{\mu+\hbar\omega_{Debye}} d\epsilon \;\; D(\epsilon) \approx D(E_F) \frac{1}{2} \int_{\mu-\hbar\omega_{Debye}}^{\mu+\hbar\omega_{Debye}} d\epsilon$$

where $D(E_F)$ is the density of states at the Fermi surface, and the factor of $1/2$ is included because the density of states includes a sum over spins and the sum over $\mathbf{k}$ does not. Using this, the gap equation (Eq. 11.27) is then rewritten as

$$1 = V_0 D(E_F) \int_{-\hbar\omega_{Debye}}^{\hbar\omega_{Debye}} d\xi \frac{1}{\sqrt{\xi^2 + \Delta^2}} = V_0 D(E_F) \text{arcsinh} \left(\frac{\hbar\omega_{Debye}}{\Delta} \right)$$

which can then be inverted to give

$$\Delta = \frac{\hbar\omega_{Debye}}{\sinh\left(\frac{1}{V_0 D(E_F)}\right)}$$

Assuming the attractive interaction V_0 is very weak, this can be approximated as

$$\Delta = 2\hbar\omega_{Debye} \exp\left(\frac{-1}{V_0 D(E_F)} \right) \tag{11.28}$$

which is extremely similar to the solution to the Cooper problem Eq. 10.18. In particular it is also non-perturbative (nonanalytic) in the strength of the interaction V_0.

> **Exercise:** An exercise worth trying is to calculate the condensation energy associated with superconductivity. This is given by
>
> $$E_{condensation} = \langle \psi_{BCS} | H_{BCS} | \psi_{BCS} \rangle - \langle FS | H_{BCS} | FS \rangle$$
>
> with $|FS\rangle$ the usual Fermi sea. If you do this correctly you will get
>
> $$E_{condensation}/V = -\frac{1}{2} D(E_F) \Delta^2 \tag{11.29}$$
>
> and we recall from Eq. 3.18 that this same quantity should also be given by
>
> $$E_{condensation}/V = \frac{1}{2} \mu_0 H_c^2 \tag{11.30}$$

It is worth looking at some of the details of the BCS wavefunction. In particular we would like to know what the functions $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ actually look like. Using Eqs. 11.22 and 11.23 we have

$$|u_{\mathbf{k}}|^2 = \sin^2 \theta_{\mathbf{k}} = \tfrac{1 - \cos 2\theta_{\mathbf{k}}}{2} = \tfrac{1}{2} \left(1 + \tfrac{\xi_{\mathbf{q}}}{\sqrt{\xi_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}} \right) \tag{11.31}$$

$$|v_{\mathbf{k}}|^2 = \cos^2 \theta_{\mathbf{k}} = 1 - \sin^2 \theta_{\mathbf{k}} = \tfrac{1}{2} \left(1 - \tfrac{\xi_{\mathbf{q}}}{\sqrt{\xi_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}} \right) \tag{11.32}$$

These functions are sketched in Fig. 11.2. Roughly v_k looks like a Fermi function — unity sufficiently far below the Fermi surface, and zero sufficiently far above. The functions only differ appreciably from 0 and 1 in a region roughly Δ around the Fermi surface. Note that in more detail this function is not like a Fermi function because the Fermi function converges exponentially to 1 and 0 whereas far from the Fermi surface whereas these converge algebraically.

How Big is a Cooper Pair?

Even if the interaction V between the electrons is very short ranged, the size of a cooper pair can be large. Let us attempt to make an estimate of this size. The important realization is that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are constant except for range of energy of roughly Δ around the Fermi surface. In terms of wavevector this means that these parameters are changing over a range of wavevectors

$$\delta k \sim \Delta / v_F$$

. Since the Fourier transform of the pair wavefunction is $g_{\mathbf{k}} \sim v_{\mathbf{k}} / u_{\mathbf{k}}$ we may conclude that the pair wavefunction has size of approximately

$$\xi_{pair} = \frac{1}{\delta k} = \frac{\hbar v_F}{\Delta}$$

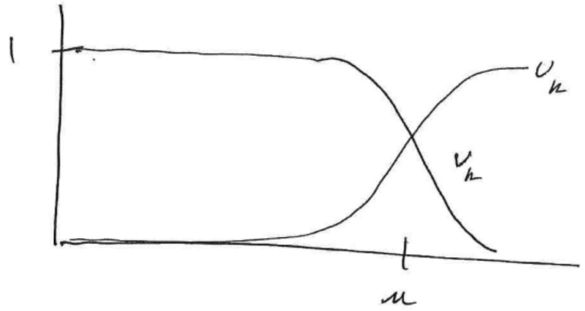

Figure 11.2: The u and v functions sketched as a function of energy (ie we plot $u_{k(E)}$ and $v_{k(E)}$

Crucially this distance can be much much larger than the distance between electrons in most metals. Thus, as expected, we do not have tightly bound pairs that can be thought of as individual bosons — as many pairs must spatially overlap with each other.

This parameter ξ_{pair} at low temperature is essentially the superconducting coherence length which we discussed in Ginzburg-Landau theory. Let us try to elucidate this connection.

To see this connection, let us equate the two expressions for the condensation energy prt unit volume given in Eq. 11.29 and 11.30

$$\frac{1}{2}D(E_F)\Delta^2 = \frac{1}{2}\mu_0 H_c^2 \tag{11.33}$$

Now recall from our discussion of Ginzburg-Landau theory that we can write H_c in terms of the London length λ and the coherence length ξ (See Eq. 6.18)

$$H_c \sim \frac{1}{\xi\lambda}\frac{\phi_0}{\mu_0}$$

where we are dropping order one factors like π and 2 for simplicity. The right hand side of Eq. 11.33 is thus

$$\frac{1}{2}\mu_0 H_c^2 \sim \frac{1}{\xi^2}\frac{1}{\lambda^2}\frac{\phi_0^2}{\mu_0} \sim \frac{1}{\xi^2}\frac{(e^*)^2 n_s}{m^*}\phi_0^2 = \frac{1}{\xi^2}\frac{\hbar^2 n_s^*}{m^*} \tag{11.34}$$

where we have used (from London theory) $\lambda^2 = m^*/((e^*)^2 n_s^* \mu_0)$ with n_s^* the superfluid density of bosons and $\phi_0 = 2\pi\hbar/e^*$) where we are still dropping order unity factors. On the other hand, on the left of Eq. 11.33 we have $D(E_F) \sim (n/E_F)$ and we set $\Delta = \hbar v_F/\xi_{pair}$ thus giving us the condensation energy (dropping order unity factors)

$$\frac{1}{2}D(E_F)\Delta^2 \sim \frac{\hbar^2 v_F^2}{\xi_{pair}^2}\frac{n}{E_F} \sim \frac{1}{\xi_{pair}^2}\frac{\hbar^2 n}{m} \tag{11.35}$$

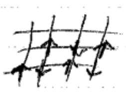

Figure 11.3: Square Latice Antiferromagnet

where we have used $E_F = \frac{1}{2}mv_F^2$. Thus up to factors of order unity (factors of 2 etc), comparing Eq. 11.34 to 11.35, and setting $n_s^* = n$ (or $n/2$) and $m^* = m$ (or $2m$) we conclude that

$$\xi_{pair} = \xi$$

the size of a Cooper pair is roughly the coherence length. However, we should be a bit cautious here that the equivalence is true at zero temperature but not near the critical temperature. We must keep in mind that in Eq. 11.34 the factor of n_s^* is the superfluid density — which is the total density at zero temperature, but goes to zero at $T = T_c$ implying that the ratio ξ/ξ_{pair} divereges as T approaches T_c.

11.3 More Exotic Pairing

The simple BCS story we have just explained can be extended in many ways. Here we will consider two interesting such extensions.

11.3.1 Anisotropic Interactions and Anisotropic Gaps: The Example of High T_c

We have assumed that the pairing interaction Eq. 11.25 and the gap function Eq. 11.26 are isotropic – i.e, they depend on the magnitude of **k** only and not on the direction of **k**. This need not be the case.

A very prominent case where interactions are expected to be anisotropic is that of the perovskite high-temperature superconductors. While there is no agreement on the detailed mechanism for superconductivity in these materials[9] there is rough general agreement on some general things. To begin with, the so-called parent compound for these material is a two-dimensional square lattice antiferromagnet (which is stabilized by strong on-site repulsive Hubbard interactions). This means that the spins are arranged in an up-down checkerboard pattern as shown in Fig. 11.3

When a small density of additional holes are added to the parent, these mobile holes run around and destroy (or "melt") the antiferromagnetic order. Nonetheless, there remains a tendency of sites neighboring each other (in vertical or horizontal direction) to have spins pointing in opposite directions — whereas spins along the diagonal tend to point in the same direction. If there is a large on-site repulsive interaction, we cannot have

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[9] Despite over 10^5 publications on the topic.

on-site pairing, and we must think about pairing between neigboring sites. If we want to make singlet pairs of electrons we should then want to make pairs in the horizontal and vertical directions (where spins point opposite), but not along the diagonal (where spins are aligned), thus implying anisotropic pairing.

In the more conventional superconductor case we discussed above, we choose out pairing function $g(\mathbf{r})$, and hence $g_{\mathbf{k}}$ to be independent of the direction of the argument. However, it is perfectly consistent to have a pairing function which depends on the direction in space. In particular, for the high T_c compounds a natural choice is to have (with $\mathbf{r} = (x, y)$

$$g(x, y) = (x^2 - y^2)\tilde{g}(r)$$

which then results analogously in

$$g_{\mathbf{k}} = (k_x^2 - k_y^2)\tilde{g}_{|k|}$$

We call this type of pairing "*d*-wave". This name comes from the name of atomic orbitals. Recall atomic orbitals are named by their angular momentum $s, p, d, f, \ldots$. This particular shape of orbital has angular momentum $L = 2$, hence is $d - wave$. As with an atom, an orbital which is isotropic in space is called s-wave. Note that we must consider only even angular momenta by fermionic (Pauli) symmetry — odd angular momenta for the spatial orbital would give us a minus sign when we exchange the two particles, and hence would require the spins to be in a triplet state (symmetric) rather than a singlet.

A model interaction which would give a d-wave pairing in 2-dimensional BCS theory is given by

$$V_{\mathbf{q},\mathbf{k}} = \left\{ \begin{array}{ll} -V_0 \cos 2\phi_{\mathbf{q}} \cos 2\phi_{\mathbf{k}} & \text{if} \qquad |\xi_{\mathbf{k}}|, |\xi_{\mathbf{q}}| < \hbar\omega_{Debye} \\ 0 & \text{otherwise} \end{array} \right. \tag{11.36}$$

which can be solved by the gap function

$$\Delta_{\mathbf{q}} = \left\{ \begin{array}{ll} \Delta \cos 2\phi_{\mathbf{q}} & \text{if} \qquad |\xi_{\mathbf{q}}| < \hbar\omega_{Debye} \\ 0 & \text{otherwise} \end{array} \right. \tag{11.37}$$

where $\phi_{\mathbf{q}}$ is the polar angle of $\mathbf{q}$ in the plane. Note that the factor of 2 in $\cos 2\phi$ shows that we have angular momentum 2.

11.3.2 Triplet Superconductors: Helium-3

So far we have only discussed condensing pairs of fermions in a singlet state. However, one can also pair fermions into a triplet state and condense those. While there are a few materials which are believed to be triplet superconductors, the most compelling case[10] of triplet pairing is that of the fermion Helium 3, which turns into a superfluid below a few hundred microkelvin in temperature[11].

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[10] Of the many thousands of materials that superconduct, perhaps 20 or so are thought to be triplets superconductors. Needless to say, these materials are pretty interesting to study.

[11] A Nobel prize was awarded in 1996 to Osheroff, Richardson, and Lee for their discovery of Helium 3 superfluidity. A Nobel prize was awareded in 2003 to Tony Leggett for theoretical understanding of this state of matter.

A simple example of a triplet superconductor is given by considering supercondcutivity in a completely spin-polarized system[12]. In this case we can write a trial wavefunction as

$$|\psi_{BCS}^{triplet}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\uparrow} \right) \tag{11.38}$$

where the pair is created with aligned spins. With fermionic symmetry we have

$$\langle c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\uparrow} \rangle = -\langle c^\dagger_{-\mathbf{k},\uparrow} c^\dagger_{\mathbf{k},\uparrow} \rangle$$

which then means that

$$\Delta_{\mathbf{q}} = -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \langle c_{-\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} \rangle = -\Delta_{-\mathbf{q}} \tag{11.39}$$

where we have only assumed $V_{\mathbf{q},\mathbf{k}} = V_{-\mathbf{q},-\mathbf{k}}$. This then implies that the spatial pairing must be antisymmetric to accomodate the symmetric pairing of the spins. An example of this is p-wave pairing

$$V_{\mathbf{q},\mathbf{k}} = \begin{cases} -V_0 \cos\phi_{\mathbf{q}} \cos\phi_{\mathbf{k}} & \text{if} \quad |\xi_{\mathbf{k}}|, |\xi_{\mathbf{q}}| < \hbar\omega_{Debye} \\ 0 & \text{otherwise} \end{cases} \tag{11.40}$$

wher e $\phi_{\mathbf{q}}$ is the angle of $\mathbf{q}$ on the Fermi surface. This type of pairing results in a gap function

$$\Delta_{\mathbf{q}} \sim \cos\phi_{\mathbf{q}}$$

Another type of p-wave pairing is the so-called "chiral" p-wave pairing, where the (complex) gap function instead takes the form

$$\Delta_{\mathbf{q}} \sim e^{i\phi_{\mathbf{q}}}$$

11.4 BCS Excitation Spectrum

Having determined the ground state of the BCS superconducting system, we now turn to ask whether we can figure out the excited states as well. Our approach is to use what is known as BCS mean-field theory, although it is essentially a small extension to Hartree-Fock.

Let us recall in Hartree-Fock theory (See Eq. 7.21) following mean field theory, we have approximated a four-fermion by taking an expectation of two of these Fermi operators and leaving the other two as operators:

$$c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \longrightarrow \quad \langle c^\dagger_\alpha c_\gamma \rangle c^\dagger_\beta c_\delta + \langle c^\dagger_\beta c_\delta \rangle c^\dagger_\alpha c_\gamma - \langle c^\dagger_\alpha c_\delta \rangle c^\dagger_\beta c_\gamma - \langle c^\dagger_\beta c_\gamma \rangle c^\dagger_\alpha c_\delta \tag{11.41}$$

In BCS theory these terms still exist, but they are not very interesting or important. They will do the same things we discussed in prior chapters: renormalize masses and so

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[12] A version of this occurs in the $\nu = 5/2$ fractional quantum Hall state

forth. Here instead we will consider some additional mean field terms that we have not previously considered

$$\langle c^\dagger_\alpha c^\dagger_\beta \rangle c_\delta c_\gamma + c^\dagger_\alpha c^\dagger_\beta \langle c_\delta c_\gamma \rangle \tag{11.42}$$

We ignored such terms previously when we studied Hartree-Fock, as the correlators must be zero for any wavefunction with a fixed number of particles. However, now that we are using the BCS trial wavefunction, where the number of particles is indefinite, these correlators are nonzero. Thus, throwing out the usual Hartree-fock terms of Eq. 11.41 but keeping the terms in Eq. 11.42, our BCS Hamiltonian Eq. 11.10 is approximated as the mean-field form

$$H_{MF} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left(\langle c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \rangle c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} + \; c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \langle c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} \rangle \right)$$

Using the expression for the gap function

$$\Delta_{\mathbf{q}} = -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle$$

we then obtain

$$H_{MF} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \sum_{\mathbf{k},\mathbf{k}'} \left(\Delta^*_{\mathbf{k}}\; c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} + \; \Delta_{\mathbf{k}}\; c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right) \tag{11.43}$$

Since this Hamiltonian is quadratic in fermion operators it is completely solvable by Bogoliubov transformation — extremely similar to what we did for bosons in section 4.5.1 above. Let us define fermionic Bogoliubon operators

$$\begin{aligned} \gamma_{\mathbf{k},\uparrow} &= u^*_{\mathbf{k}} c_{\mathbf{k},\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k},\downarrow} \\ \gamma^\dagger_{-\mathbf{k},\downarrow} &= v^*_{\mathbf{k}} c_{\mathbf{k},\uparrow} + u_{\mathbf{k}} c^\dagger_{-\mathbf{k},\downarrow} \end{aligned} \tag{11.44}$$

It is easy to check that this set of operators satisfies fermionic canonical commutations relations

$$\{\gamma_{\mathbf{k},\sigma}, \gamma^\dagger_{\mathbf{k}',\sigma'}\} = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} \tag{11.45}$$

$$\{\gamma_{\mathbf{k},\sigma}, \gamma_{\mathbf{k}',\sigma'}\} = \{\gamma^\dagger_{\mathbf{k},\sigma}, \gamma^\dagger_{\mathbf{k}',\sigma'}\} = 0 \tag{11.46}$$

With some algebra, once can check that the mean-field Hamiltonian then can be rewritten as

$$H_{MF} = \text{Ground State Energy} + \sum_{\mathbf{k},\sigma} E_{\mathbf{k}}\; \gamma^\dagger_{\mathbf{k},\sigma} \gamma_{\mathbf{k},\sigma} \tag{11.47}$$

where the (positive) Bogoliubon energy is

$$E_{\mathbf{k}} = +\sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} \tag{11.48}$$

Exercise: The algebra involved in showing that Eq. 11.47 is the same as Eq. 11.43 is tedious but straightfoward — one simply substitutes the expressions for γ and $\gamma^\dagger$ in terms of c and $c^\dagger$ as given in Eq. 11.44 into Eq. 11.47. It is worth working through this as an exercise. To get you started, we will try deriving a particular term on the right of Eq. 11.43, the kinetic term with spin $\uparrow$. We will make the desired substitution and only keep track of terms where there is exactly one $c_{\mathbf{k},\uparrow}$ and one $c^\dagger_{\mathbf{k},\uparrow}$ and throw out all other terms.

$$\begin{aligned} & E_{\mathbf{k}}\left(\gamma^\dagger_{\mathbf{k},\uparrow}\gamma_{\mathbf{k},\uparrow} + \gamma^\dagger_{-\mathbf{k},\downarrow}\gamma_{-\mathbf{k},\downarrow}\right) \\ = \;& E_{\mathbf{k}}\Big((u_{\mathbf{k}}c^\dagger_{\mathbf{k},\uparrow} - \ldots)(u^*_{\mathbf{k}} - \ldots) + (v^*_{\mathbf{k}}c_{\mathbf{k},\uparrow} + \ldots)(v_{\mathbf{k}}c^\dagger_{\mathbf{k},\uparrow} + \ldots)\Big) \\ = \;& E_k\left(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2\right) c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow} + \text{const} \end{aligned}$$

The factor $(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) = \sin^2\theta_{\mathbf{k}} - \cos^2\theta_{\mathbf{k}} = -\cos 2\theta_{\mathbf{k}}$ from Eq. 11.16. Then using Eq. 11.22 (and finally Eq. 11.48) our expression becomes

$$\begin{aligned} = \;& E_k\left(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2\right) c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow} + \text{const} = E_k\cos 2\theta_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow} \\ = \;& \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}\left(\frac{\xi_{\mathbf{k}}}{\sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}}\right) c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow} = \xi_{\mathbf{k}} c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow} \end{aligned}$$

which is exactly the term we expect in Eq. 11.43.

Having derived the mean field Hamitlonian Eq. 11.47 and the spectrum Eq. 11.48 we note that the BCS ground state is the state is simply the Bogoliubov vacuum

$$\gamma_{\mathbf{k},\sigma}|\psi_{BCS}\rangle = 0$$

and excitations of (always nonnegative) energy E_k are created by the operator $\gamma^\dagger_{\mathbf{k},\sigma}$.

Let us think a bit more carefully about the structure of these quasiparticles . First, the quasiparticle in Eqs. 11.44 is a superposition of an electron and a hole. As $\xi_{\mathbf{k}}$ gets much larger than zero (looking at the structure of u and v as shown in Eq. 11.2) the quasiparticle operator $\gamma^\dagger$ becomes mostly an electron creation operator (and only a tiny bit of a hole creation). Whereas when ξ becomes much less than zero, the quasiparticle operator is mostly a hole creation operator and only a little bit of an electron creation operator.

Let us consider the simple isotropic (s-wave) case we have considered in Eq. 11.26 where Δ is just a constant indpendent of direction on the Fermi surface. In this case, the minimum energy excitation (Eq. 11.47) is of energy Δ, hence the name “gap” assigned to the paramter Δ.

The existence of the energy gap has a number of profound ramifications. For example, due to the lack of low energy excitations, the electronic heat capacity goes to zero exponentially at low temperature roughly as $e^{-\Delta/T}$. Similarly electronic thermal transport, and electronic ultrasonic attenuation[13] drop exponentially at low temperature. Another classic experiment is known as Knight shift, which measures the spin susceptibility (how easy it is to flip a spin). For singlet superconductors[14], at low temperature when there are no quasiparticles present, the Knight shift drops to zero, since to flip a spin one needs to break a pair.

Finally we note that the absence of low energy excitations assures that a superconductor satisfies the Landau criterion for superfluidity!

Density of States

It is useful to try to figure out the density of states in a superconductor (again assuming the simple s-wave form). The easiest way to do this is to always go back to the density of states in $\mathbf{k}$ space which is completely fixed by the volume of the system. As usual, let the nonsuperconducting kinetic energy of an electron be called $\xi = \hbar^2 k^2/(2m) - \mu$ (we then convert k-space integrals to energy integrals as

$$2V \int \frac{d^3k}{(2\pi)^3} \ldots = \int d\xi D_N(\xi) \ldots$$

with $D_N(\xi)$ the normal-state density of states. Near the Fermi surface, $D_N(\xi)$ can be approximated as a constant density of states, which we usually call $D(E_F)$.

Similarly, however, we could write this as an integral over the energy of the superconducting quasiparticles

$$= \int dE D_S(E) \ldots$$

where $D_S(E)$ is the density of states of superconducting quasiparticles. Thus we have the relation

$$D_S(E)dE = D_N(\xi)d\xi \approx D(E_F)d\xi$$

or equivalently

$$D_S(E) = D(E_F)\frac{d\xi}{dE}$$

Using Eq. 11.48 we have

$$\xi = \sqrt{E^2 - \Delta^2}$$

where we have assumed the isotropic s-wave case where Δ is just a constant. We then have

$$D_S(E) = D(E_F)\frac{E}{\sqrt{E^2 - \Delta^2}} \qquad E > \Delta$$

as sketched in Fig. 11.4. We see that the states that had energy below Δ in the normal state are pushed up above Δ to form a peak in the superconducting density of states. This

---

[13] In ultrasonic attenuation, sound is sent through a metal – the energy of the sound wave can be absorbed by the electrons in the system (if there is no energy gap) thus attenuating the sound.

[14] For triplet superconductors one can smoothly rotate the spin of the pair without breaking the pair and the Knight shift does not drop to zero at low temperature.

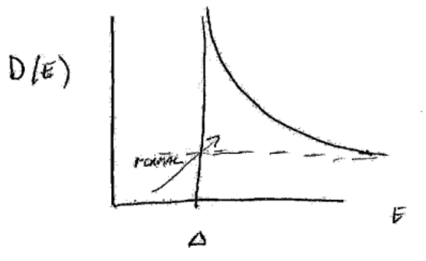

Figure 11.4: The density of states of a superconductor.

density of states is easily measured in tunneling experiments where one tunnels unpaired electrons into the superconductor.

11.5 Finite Temperature Gap Equation

At finite temperature the quasiparticles can be thermally excited. We should expect that

$$\langle \gamma^\dagger_{\mathbf{k},\sigma} \gamma_{\mathbf{k},\sigma} \rangle = n_F(E_k)$$

where n_F is the Fermi function

$$n_F(x) = \frac{1}{e^{\beta x} + 1}$$

We can then think of the system at finite temperature as having the γ states thermally occupied. However, the occupation of these thermal states will then have a feedback effect on the gap function itself.

To see how this happens, we re-do the calculation of the gap function of Eq. 11.20 but now at finite temperature. To do this we need to invert Eq. 11.44 to write c and $c^\dagger$ in terms of γ as follows

$$\begin{aligned} c_{-\mathbf{k},\downarrow} &= -v_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}\uparrow} + u^*_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow} \\ c^\dagger_{\mathbf{k},\uparrow} &= u^*_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow} \end{aligned}$$

Then plugging into Eq. 11.20 we get

$$\begin{aligned} \Delta_{\mathbf{q}} &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle && (11.49) \\ &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} u^*_{\mathbf{k}} v_{\mathbf{k}} \langle 1 - \gamma^\dagger_{-\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\uparrow} - \gamma^\dagger_{\mathbf{k}\downarrow} \gamma_{\mathbf{k}\downarrow} \rangle && (11.50) \end{aligned}$$

where we have dropped terms like $\gamma^\dagger_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\downarrow}$ since they will give zero in a sector with a fixed

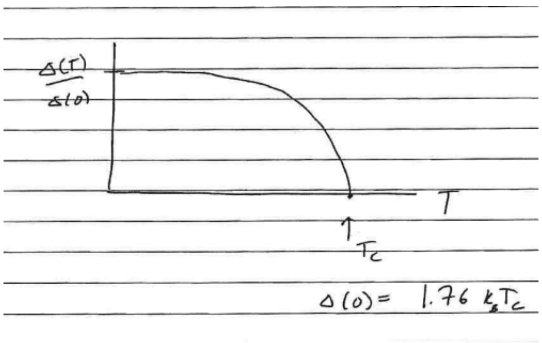

Figure 11.5: Gap as a function of T

occupation of quasiparticles. We then have

$$\begin{aligned}
\Delta_{\mathbf{q}} &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} u^*_{\mathbf{k}} v_{\mathbf{k}} (1 - 2n_F(E_k)) && (11.51)\\
&= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} (1 - 2n_F(E_k)) && (11.52)
\end{aligned}$$

where we have used that $2u^*_{\mathbf{k}} v_{\mathbf{k}} = \sin 2\theta_{\mathbf{q}}$ along with Eq. 11.23.

With the same assumption of isotropic interaction, and isotropic gap function (Eqs. 11.25 and 11.26) we obtain a modified version of the BCS gap equation that includes a thermal occupation factor (here using that $1 - 2n_F(x) = \tanh(x/2)$) given by

$$\begin{aligned}
1 &= \frac{V_0}{2} \sum_{\substack{\mathbf{k} \\ \xi_{\mathbf{k}} < \hbar\omega_{Debye}}} \frac{\tanh\left(\frac{1}{2}\beta\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}\right)}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} \\
&= \frac{V_0 D(E_F)}{2} \int_{-\omega_{Debye}}^{\omega_{Debye}} d\xi \, \frac{\tanh\left(\frac{1}{2}\beta\sqrt{\xi + \Delta^2}\right)}{\sqrt{\xi^2 + \Delta^2}} && (11.53)
\end{aligned}$$

where we have converted the sum over $\mathbf{k}$ to an integral over energy analogous to the discussion after Eq. 11.24. This equation now implicitly defines the gap Δ as a function of temperature ($\beta = 1/k_b T$). While the integral is not possible to do analytically, it can be done numerically to give a dependency roughly as that shown in Fig. 11.5. At some temperature, which we now define as T_c, the gap Δ goes to zero and above this temperature there is no solution. Further, the ratio of $k_B T_c$ to the gap at zero temperature is a universal constant

$$\Delta(T = 0) = 1.76\, k_B T_c$$

a relationship that holds true reasonably well in most conventional superconductors.

11.6 Inhomogeneous Superconductors

So far we have only studied superconductors in clean systems where $\mathbf{k}$ is a good quantum number. However, this is not necessary. Let us introduce some amount of disorder $U(\mathbf{r})$ and write a single-particle Hamiltonian as

$$\hat{h} = \frac{-\hbar^2\nabla^2}{2m} + U(\mathbf{r}) - \mu \tag{11.54}$$

We can then write a more general effective Schroedinger equation in real-space as

$$\begin{pmatrix} \hat{h} & \Delta(\mathbf{r}) \\ -\Delta^*(\mathbf{r}) & -\hat{h}^* \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}$$

which is known as the Bogoliubov-de Gennes equation. This is supplemented by the real-space definition of the gap function

$$\Delta(\mathbf{r}) = -V_0 \sum_n u_n(\mathbf{r}) v_n(\mathbf{r})$$

In the translationally invariant case these equations are equivalent to the above discussion. However, they also allow for disordered eigenfunctions as well. We can similarly define quasiparticle operators which then take the real-space form such as

$$\gamma_{n\uparrow} = \int d\mathbf{r} \left(\hat{\psi}^\dagger(\mathbf{r})_\uparrow u_n^*(\mathbf{r}) - v_n(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \right)$$

analogous to the momentum space version in Eq. 11.44.

An important theorem due to Anderson (creatively called "Anderson's theorem") states that weak (nonmagnetic) disorder added in Eq. 11.54 does not reduce the size of the gap or reduce the critical temperature. This is the reason that superconductivity can survive disorder. The essence of this theorem is that (at least in non-magnetic systems –i.e., systems that obey time reversal invariance) it is always possible to pair an electron with its time reversed partner. In the absence of disorder we pair $\mathbf{k}\uparrow$ with $-\mathbf{k}\downarrow$. When we break translational invariance we may not have $\mathbf{k}$ states any more, but nonetheless we can pair an eigenstate with its time-reversed partner.

11.7 Ginzburg-Landau, Number-Phase, and Josephson

Since the gap parameter vanishes at the critical temperature, it is natural to ask what its relationship is to the Ginzburg-Landau order parameter introduced in section 6.2. Indeed, these can be roughly considered to be the same thing (once we include an appropriate normalization, they become equivalent). We can go a step further and ask about the phase of the order parameter.

The superconductor can be given an arbitrary complex phase in the same way we would introduce a phase for a neutral superfluid or a coherent state (See for example, section 4.1.2). For a neutral superfluid, we would write

$$e^{|\alpha| e^{i\varphi} a^\dagger}|0\rangle$$

Applying the same philosophy here, we obtain a BCS wavefunction of the form

$$|\psi_\varphi\rangle = \prod_k \left(|u_k| + e^{i\varphi}|v_k| c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right) \tag{11.55}$$

As with the coherent state in section 4.1.2, since each pair comes with a factor of $e^{i\varphi}$ (just like with a coherent state) the action of $-i\partial/\partial\varphi$ and the action of the number operator $\hat{N}$ which counts pairs are equivalent. Thus we have[15]

$$-i\frac{\partial}{\partial\varphi} = \hat{N} \tag{11.56}$$

and conversely

$$i\frac{\partial}{\partial N} = \varphi \tag{11.57}$$

from which we also have

$$e^{-i\varphi} = e^{\frac{\partial}{\partial N}} = \hat{N}^{+} \tag{11.58}$$

which is a shift operator which increase the value of N by one[16]. For example, consider the pair creation operator in Eq. 11.13. We see that this has value $v^* u$, which in Eq. 11.55 is indeed proportional to $e^{-i\varphi}$.

We can check that this additional phase included in Eq. 11.55 is reflected in the gap function by using Eq. 11.19

$$\begin{aligned}\Delta_{\mathbf{q}} &= -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}}\, u^*_{\mathbf{k}} v_{\mathbf{k}} = -\sum_{\mathbf{k}} V_{\mathbf{q},\mathbf{k}}\, |u_{\mathbf{k}}||v_{\mathbf{k}}| e^{i\varphi} \\ &= \Delta^0_{\mathbf{q}}\, e^{i\varphi}\end{aligned}$$

We can check that no energies depend on the overall phase, since this is just a gauge degree of freedom as expected. However relative phases are physical quantities.

11.7.1 Josephson Effect

Let us now consider two superconductors connected by a voltage meter as shown in Fig. 11.6 The BCS wavefunction of each superconductor has an indefinite number of par-

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[15] Compare these to the conjugate pair $p = -id/dx$ and $x = id/dp$.

[16] To see this note that $e^{d/dx}$ is an operator that when applied to a function $f(x)$ returns $f(x+1)$. This is demonstrated by expanding the exponential and recognizing it as a Taylor series

$$e^{d/dx} f(x) = \left(1 + \frac{d}{dx} + \frac{1}{2}\frac{d^2}{dx^2} + \ldots\right) f(x) = f(x+1)$$

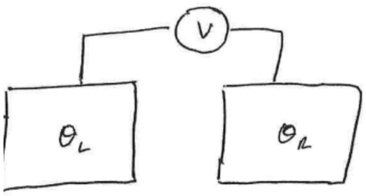

Figure 11.6: this is the caption

ticles, but has a definite phase. Recalling that the Hamiltonian is actually a free energy (since energy is measured with respect to the chemical potential μ, see footnote in section 11.2). This means that adding a pair into the condensate does not generally increase or decrease the free energy. However, once we add a voltage between two superconductors, then transferring a pair from one superconductor to the other does cost energy. Thus we can write an effective Hamiltonian of the form

We can represent their effective Hamiltonians as

$$H_{eff} = -eV(\hat{N}_L - \hat{N}_R)$$

where $\hat{N}_{L,R}$ is the number of pairs on the left, or right respectively (note that transferring a pair from left to right changes the energy by $2eV$ as it should). Using the Heisenberg equations of motion to determine the evolution of the difference in the phases of hte two superconductors we have

$$i\hbar\frac{\partial(\varphi_L - \varphi_R)}{\partial t} = [(\varphi_L - \varphi_R), H] = [(\varphi_L - \varphi_R), -eV(\hat{N}_L - \hat{N}_R)]$$

Now using Eq. 11.56 we obtain

$$i\hbar\frac{\partial(\varphi_L - \varphi_R)}{\partial t} = -eV\left[(\varphi_L - \varphi_R)\,,\,(-i\frac{\partial}{\partial\varphi_L} + i\frac{\partial}{\partial\varphi_R})\right]$$

or

$$\frac{\partial(\varphi_L - \varphi_R)}{\partial t} = \frac{-2eV}{\hbar} \tag{11.59}$$

This conversion of voltage into frequency is used metrologically to fix the definition of the volt.

If we now set the voltage between the two sides to zero, and let current flow between the two sides, let us ask how the current depends on the phases of the two sides. Here, we argue by analogy. Number and phase are conjugate variables analogous to momentum and position. Let us recall Hamilton's equations for momentum and position

$$\frac{\partial H}{\partial p} = \frac{\partial x}{\partial t} \tag{11.60}$$

$$\frac{\partial H}{\partial x} = -\frac{\partial p}{\partial t} \tag{11.61}$$

Now replace the conjugate variables x and p with $\varphi_L - \varphi_R$ and $N_L - N_R$. We then have

$$\frac{\partial H}{\partial(\varphi_L - \varphi_R)} = -\frac{\partial(N_L - N_R)}{\partial t} \tag{11.62}$$

$$\frac{\partial H}{\partial(N_L - N_R)} = \frac{\partial(\varphi_L - \varphi_R)}{\partial t} \tag{11.63}$$

The latter of these two equations we immediately identify as giving us exactly Eq. 11.59. The former of these two equations, instead gives us

$$\langle J \rangle = 2e \frac{\partial \langle H \rangle}{\partial(\varphi_L - \varphi_R)} \tag{11.64}$$

with J the current between the two subsystems. We thus must determine how the energy of the two superconductors depend on their phases. Since within each subsystem, the phase is a gauge degree of freedom, the overall dependence on the relative phase can only come from the coupling between the two subsystems which we assume is weak. Let us focus on this coupling. We write a tunneling Hamiltonain beween the two systems as follows

$$H_{tun} = \hat{t} + \hat{t}^\dagger$$

where $\hat{t}$ tunnels a single electron from right to left. More explicitly we can write

$$\hat{t} = \sum_{\mathbf{k},\mathbf{q},\sigma} T_{k,q} c^\dagger_{L\mathbf{k},\sigma} c_{R,\mathbf{q},\sigma}$$

We now treat the coupling order by order in perturbation theory. At first order in perturbation theory we have

$$\delta E_1 = \langle H_{tun} \rangle = 0$$

The reason for this is that the ground state has an even number of electrons on both side. Applying H_{tun} once will put an odd number on both sides thus being orthogonal to the ground state.

At second order in perturbation theory, we have the following (written in a bit of shorthand)

$$\begin{aligned}\delta E_2 = &\sum_m \frac{\langle GS|\hat{t}^\dagger|m\rangle\langle m|\hat{t}|GS\rangle}{E_0 - E_m} + \sum_m \frac{\langle GS|\hat{t}|m\rangle\langle m|\hat{t}^\dagger|GS\rangle}{E_0 - E_m} \\ &+ \sum_m \frac{\langle GS|\hat{t}|m\rangle\langle m|\hat{t}|GS\rangle}{E_0 - E_m} + \sum_m \frac{\langle GS|\hat{t}^\dagger|m\rangle\langle m|\hat{t}^\dagger|GS\rangle}{E_0 - E_m}\end{aligned}$$

where $|GS\rangle$ indicates the BCS ground state on both sides, and $|m\rangle$ is some excitation where a single electron is moved from one side to the other, leaving a broken pair on both sides. The terms on the first line move a particle from one side to the other and then move it back from where it came in order to get back into the ground state — implying no net motion of electrons from one side to the other. On the other hand, the terms on the second line transfer a pair of electrons either left to right or right to left. By Eq. 11.58 these terms must be proportional to $e^{i(\varphi_R - \varphi_L)}$ or $e^{i(\varphi_L - \varphi_R)}$ respectively. Thus we have

$$\delta E_2 = \mathrm{Const} + X e^{i(\varphi_R - \varphi_L)} + X^* e^{i(\varphi_L - \varphi_R)}$$

with X some complex constant. We can argue that for a system with no time reversal breaking, all matrix elements should be real (in the absence of a complex superconducting phase). This allows us to conclude thta X should be real and we obtain

$$\delta E_2 = \mathrm{Const} + 2X \cos(\varphi_R - \varphi_L)$$

Hence using Eq. 11.64 we have

$$\langle J \rangle = I_c \sin(\varphi_R - \varphi_L)$$

with $I_c = 4eX$ known as the critical current. This relationship between tunnelling current and superconducting phase difference is known as the DC-Josephson effect[17]. Roughly one can think of this as the discrete analog of supercurrent being given as the gradient of the phase.

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[17] Predicted by Josephson when he was 22 years old in 1962. He won a Nobel prize eleven years later. Most of his life after the Nobel prize has been devoted to studying what other scientists term "fringe" theories — including topics such as meditation, telepathy, higher states of consciousness, parapsychology and so forth.

Chapter 12

An Introduction to Majoranas

The hunt for Majoranas[1] has been an obsession of the condensed matter community for over a decade. While several recent experiments, in a number of different experimental systems, have been extremely suggestive that the elusive Majorana has been found, for the sceptics definitive proof is still awaited.

This chapter introduces the concept of Majoranas, how they may appear, and why they are so interesting.

Let us begin by recalling our definition of fermionic operators from Eq.12.2:

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \tag{12.1}$$

$$\{c_i, c_j^\dagger\} = \delta_{ij} \tag{12.2}$$

We will now be more specific and call these fermionic operators *Dirac* fermions. The Hilbert space associated with a given Fermion orbital j is two dimensional, it can be either empty, which we notate as $|0_j\rangle$ or filled which we notate as $|1_j\rangle$. The filled and empty states can be transformed into each other by applying the Dirac fermion operators.

$$c_j^\dagger|0_j\rangle = |1_j\rangle \qquad c_j|1_j\rangle = |0_j\rangle.$$

Ettore Majorana[2] found a way to to constructed fermionic operators that are their own Hermitian conjugates. We can construct such operators from the Dirac fermion operators. For a set of Fermion orbitals $j = 1, 2, \ldots N$, let us define so-called Majorana

---

[1] "Majorana" is pronounced roughly my-or-ah-nah. I've heard Italians argue over how you should or should not emphasize the syllables.

[2] Majorana was a young genius who dissapeared off the face of the earth in 1938 at the young age of 32. There are many theories as to what happened to him. Some say he committed suicide by jumping off a ship. Others say he ran afoul of the Mafia and is at the bottom of the ocean with cement shoes. Still others think he escaped to South America to start his life over under another name. Due to the extensive recent interest in Majorana, the Rome attorney's office released a statement in 2015 saying that the believe he had moved to Venezuela. They then declared the case closed.

operators

$$\begin{aligned}
\gamma_1 &= (c_1^\dagger + c_1) & \gamma_2 &= i(c_1^\dagger - c_1) \\
\gamma_3 &= (c_2^\dagger + c_2) & \gamma_4 &= i(c_2^\dagger - c_2) \\
& \vdots & & \qquad (12.3) \\
\gamma_{2N-1} &= (c_N^\dagger + c_N) & \gamma_{2N} &= i(c_N^\dagger - c_N) \qquad (12.4)
\end{aligned}$$

Notice that these Majorana operators are their own Hermitian conjugates

$$\gamma_j^\dagger = \gamma_j$$

This essentially means that the Majorana describes a particle that is its own anti-particle. It is easy to check that the anti-commutation relations of the Majorana operators are

$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}$$

and in particular this means that

$$\gamma_i^2 = 1$$

Note that the γ operators change the particle number in an indefinite way — they are a superposition of creating and annihilating a fermion. In both cases, the parity of the number of femions is changed. Given our discussion of quasiparticles in superconductors, this should now not look so unusual.

Note that Majoranas always come in pairs[3]. Since the number of fermion orbitals in a system is an integer, if we convert to Majorans we will always have an even number of Majoranas. .

The tranformation from Dirac fermions to Majoranas can of course be inverted. A system of $2N$ Majoranas can be converted into Dirac fermion via

$$\begin{aligned}
c_1^\dagger &= \frac{1}{2}(\gamma_1 - i\gamma_2) & c_1 &= \frac{1}{2}(\gamma_1 + i\gamma_2) \\
c_2^\dagger &= \frac{1}{2}(\gamma_3 - i\gamma_4) & c_2 &= \frac{1}{2}(\gamma_3 + i\gamma_4) \\
& \vdots & & \\
c_N^\dagger &= \frac{1}{2}(\gamma_{2N-1} - i\gamma_{2N}) & c_N &= \frac{1}{2}(\gamma_{2N-1} + i\gamma_{2N}) \qquad (12.5)
\end{aligned}$$

In partiuclar note that the number operator for one of these orbitals (say the first orbital) is given by

$$\hat{n}_1 = c_1^\dagger c_1 = \frac{1}{2}(1 + i\gamma_1\gamma_2)$$

meaning that the operator $i\gamma_1\gamma_2$ has eigenvalues ±1 corresponding to filled or empty orbitals respectively

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[3] Like the Sith.

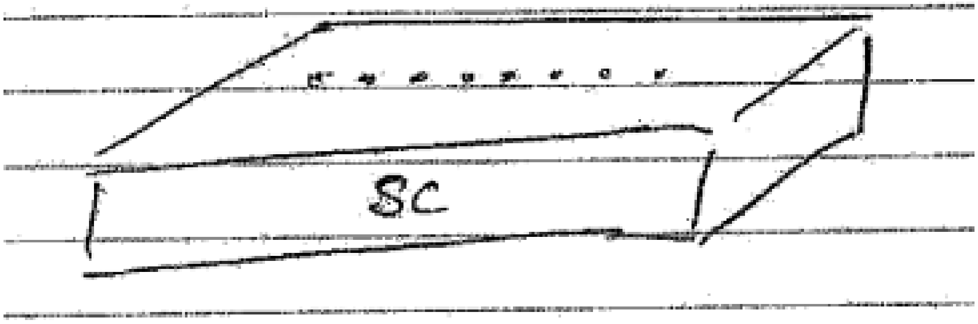

Figure 12.1: The KitaevWire. Individual sites arranged in a wire on the surface of a spinless superconductor

It is important to note that we cannot say that a single Majorana is filled or empty the same way we can say this for a regular Dirac fermion orbital. In order to say something is filled or empty we must put two Majorana operators together in pairs in order to make Dirac fermions, whose orbitals can be filled or empty. (As we will discuss further below, we have choices in how we choose to pair these Majorana operators to make Dirac fermions.)

Since we can tranform from N Dirac fermions to $2N$ Majoranas, any Hamiltonian that we can write in terms of Dirac fermions (such as the interacting fermion Hamiltonians from chapter 7. See section 7.2.3 for example) can be written equally well in terms of Majoranas. So far we haven't done anything except re-express the same Hamiltonian in a different language. However, soon we will give interesting physical meaning to the individual Majoranas!

12.1 The Kitaev Chain

The explosion of interest in Majoranas was perhaps spurred by a pivotal paper by Alexei Kitaev in 2000[4]. This chapter will summarize much of that work.

Let us consider a bulk (fully gapped) superconductor of *spinless* fermions (or more realistically, spin polarized fermions, so we can forget about the spin degree of freedom). As discussed in section 11.3.2 for spinless electrons, we need to have triplet pairing such as chiral p-wave (we need chiral so that the superconductor is gapped in all directions on the Fermi surface). This is not much more complicated than singlet pairing. Now, on the surface of this superconductor, let us put a number N of sites where these spinless fermions may sit — and we arrange these sites into a one-dimensional wire as shown in Fig. 12.1.

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[4] See arXiv:cond-mat/0010440

The Hamiltonian for this wire is given as

$$\begin{aligned} H &= \sum_{j=1}^{N-1} -t(c^\dagger_{j+1} c_j + c^\dagger_j c_{j+1}) \\ &+ \sum_{j=1}^{N} -\mu(c^\dagger_j c_j - \frac{1}{2}) \\ &+ \sum_{j=1}^{N-1} \Delta_j c^\dagger_j c^\dagger_{j+1} + \Delta^*_j c_j c_{j+1} \end{aligned} \tag{12.6}$$

The first term is the usual hopping term whereby a ferrmion hops from one site to the neighboring site. The second term is just a chemical potential term — with a shift in energy so that at $\mu = 0$ is particle-hole symmetric. Finally the last term is the interesting one —which looks like a pairing term in a Bogoliubov-de Gennes Hamiltonian. In this context, this term creates or annihilates fermions on the chain in pairs. In fact what this is representing is that fermions can jump on and off of the chain in pairs into the bulk superconductor. They cannot jump one at a time because that would give an odd number of fermions in the superconductor which would require breaking a pair and would cost the energy gap in the superconductor (which we assume is large). Note that this term creates or annihilates fermions at neighboring sites of the chain: We cannot put two fermions on the same site of the chain because of the Pauli principle.

For simplicity let us assume that the gap function Δ is homogenious in space

$$\Delta_j = \Delta = |\Delta| e^{i\theta}$$

although being independent of position is not required.

Now this Hamiltonian is quadratic in fermion operators, so it can be solved by Bogoliubov transform. (Maybe add an appendix doing this?). However, it is more instructive to look at a few special cases to understand what can happen. Before doing this, it is useful to transform this Hamiltonian to its Majorana representation:

To do this we transform

$$\begin{aligned} \gamma_{2j-1} &= e^{-i\theta/2} a^\dagger_j + e^{i\theta/2} c_j \\ \gamma_{2j} &= i e^{-i\theta/2} a^\dagger_j - i e^{i\theta/2} c_j \end{aligned}$$

This is exaclty the same as the tranform of Eq. 12.4 except that we have absorbed the phase of the gap function θ to simply the result. With this transform we obtain the Hamiltonian

$$\begin{aligned} H &= \frac{-\mu}{2}\sum_{j=1}^{N} i\gamma_{2j-1}\gamma_{2j} \\ &+ \frac{(|\Delta|+t)}{2}\sum_{j=1}^{N-1} i\gamma_{2j}\gamma_{2j+1} \\ &+ \frac{(|\Delta|-t)}{2}\sum_{j=1}^{N-1} i\gamma_{2j-1}\gamma_{2j+2} \end{aligned} \tag{12.7}$$

Again this is quadratic in fermion operators and is therefore solvable analytically. However, instead let us look at some simple cases.

Case 1: $t = \Delta = 0$

In this case the Hamiltonian is simply

$$H = \frac{-\mu}{2}\sum_{j=1}^{N} i\gamma_{2j-1}\gamma_{2j} = \sum_{j=1}^{N} -\mu(c_j^\dagger c_j - \frac{1}{2})$$

The ground state is simply to fill all the orbitals with a fermion, or leave them all empty, depending on the sign of μ.

Case 2: $\mu = 0$ **and** $|\Delta| = t$

This is a more interesting case. Here the Hamiltonian is just

$$H = t\sum_{j=1}^{N-1} i\gamma_{2j}\gamma_{2j+1}$$

To solve this Hamiltonian, we need to assemble the Majorana operators γ into Dirac fermions. But these fermions are *not* the original Dirac fermions c_j and $c_j^\dagger$ but instead different linear combinations. Let us define

$$\begin{aligned} \tilde{c}_1^\dagger &= \frac{1}{2}(\gamma_2 - i\gamma_3) & \tilde{c}_1 &= \frac{1}{2}(\gamma_2 + i\gamma_3) \\ \tilde{c}_2^\dagger &= \frac{1}{2}(\gamma_4 - i\gamma_5) & \tilde{c}_2 &= \frac{1}{2}(\gamma_4 + i\gamma_5) \\ &\vdots \\ \tilde{c}_{N-1}^\dagger &= \frac{1}{2}(\gamma_{2N-2} - i\gamma_{2N-1}) & \tilde{c}_{N-1} &= \frac{1}{2}(\gamma_{2N-2} + i\gamma_{2N-1}) \end{aligned} \tag{12.8}$$

In terms of these new Dirac fermions we have

$$H = 2t\sum_{j=1}^{N-1}(\tilde{c}_j^\dagger \tilde{c}_j - \frac{1}{2})$$

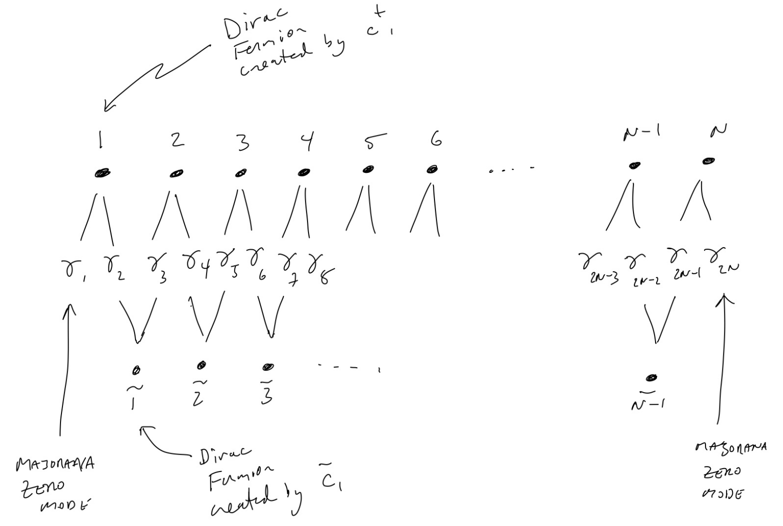

Figure 12.2: Here we show

The ground state of this is to either fill all of the new tilde Dirac fermion orbitals or leave them all empty depending on the sign of t.

What we have done here is depicted in Fig. 12.2. Originally the Majoranas γ_1 and γ_2 come from the first Dirac fermion site, but then we re-assemble new Dirac fermions out of γ_2 and γ_3.

What is interesting here is that there are two remaining Majoranas that are left over at the end of this transformation and are not reassembled into the tilde Dirac fermions. These two Majoranas, γ_1 and γ_{2N} do not enter into the Hamiltonian. We can assemble these two remaining Majoranas into a single Dirac fermion via

$$f^\dagger = \frac{1}{2}(\gamma_1 - i\gamma_{2N}) \qquad\qquad f = \frac{1}{2}(\gamma_1 + i\gamma_{2N})$$

where, since it does not enter the Hamiltonian, the energy of the system is indepdendent of whether this Dirac fermion is in the occupied or unoccupied state. Since this mode is zero energy, the two Majorana γ_1 and γ_{2N} are known as *Majorana zero modes.*

The two states of the system, corresponding to having the f orbital filled or empty differ in fermion parity but not in energy. It is interesting, and important, that this two state system is *delocalized* between the two ends of the system – which can be arbitrarily far apart.

The excitement over Majoranas is partially due to the their potential use for quantum computation and quantum information processing — a feature first pointed out by Kitaev. The general idea is to use this type of two-state system as a quantum bit (or qubit). We will see that, although this might look like an inconvenient two-state system, there are significant advantages to storing information this way.

The obvious question to ask is whether we obtained zero modes simply because we fine-tuned our Hamiltonian, setting $\mu = 0$ exactly and $t = |\Delta|$ exactly (and dropping any term that is not of the form of .Eq. 12.6 such as four fermi terms). I claim that for a wide range of parameters (not fine-tuned), we will still have Majorana zero modes, although the solution of the Hamiltonian is not as simple. We will give two approaches to analyzing the system

12.1.1 Bogoliubov Approach

As mentioned above, since the Hamiltonian Eq. 12.6 is quadratic in Fermi operators it is always solvable by Bogoliubov transformation. reults:

Bulk spectrum: For an infinitely long chain we have a spectrum of excitations

$$E(q) = \pm\sqrt{(2t\cos q + \mu)^2 + 4|\Delta|^2 \sin^2 q}$$

This calculation is left as a challenge for the reader (or maybe I add an appendix?). This spectrum has gapless excitations only when $\Delta = 0$ or $|2t| = |\mu|$, otherwise the spectrum is completely gapped. We can identify

ADD MORE HERE